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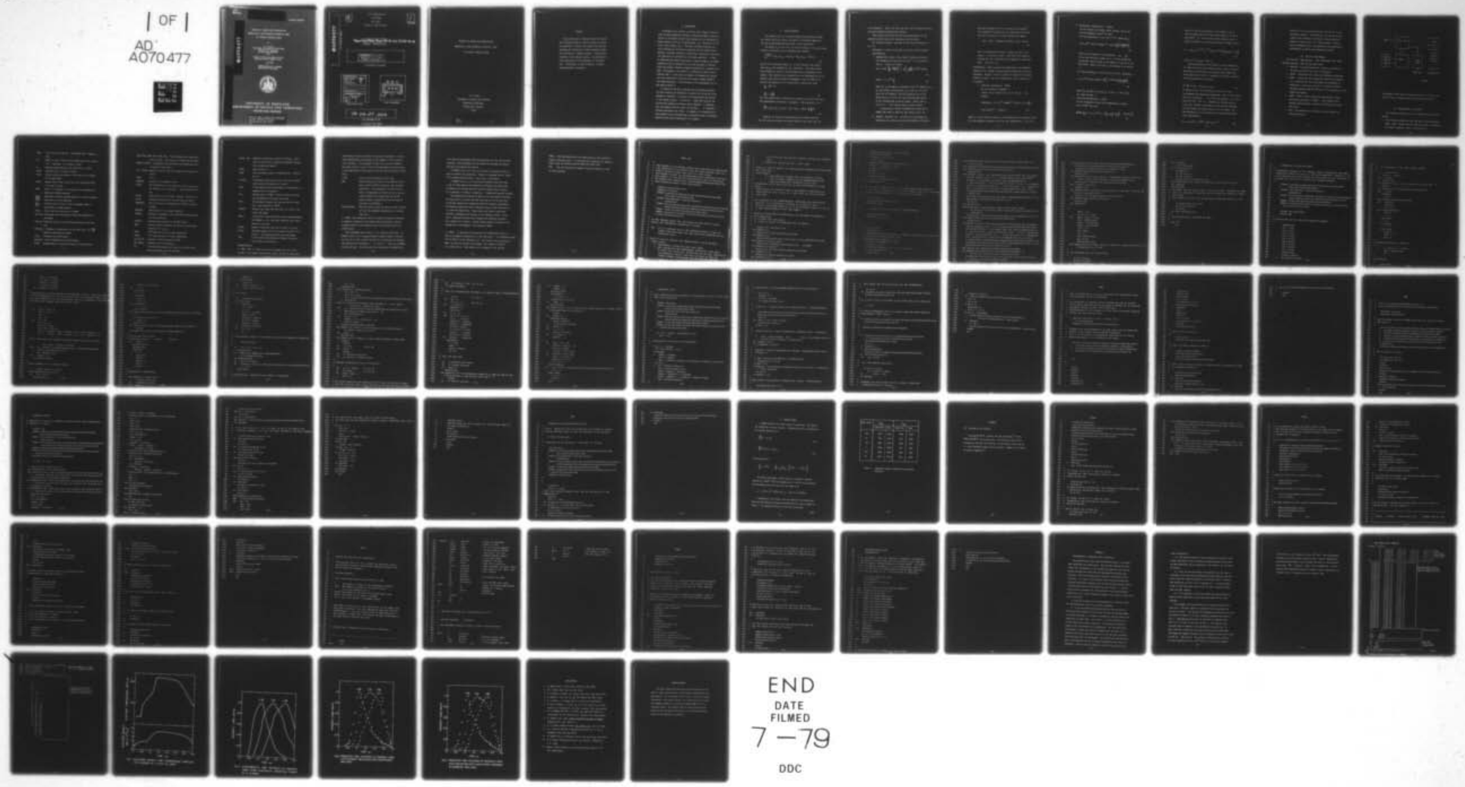

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SOLUTION OF COUPLED RATE EQUATIONS AND PREDICTION OF TIME HISTORIES OF EMISSION LINES IN A RAPIDLY IONIZING PLASMA

by

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SOLUTION OF COUPLED RATE EQUATIONS AND PREDICTION OF TIME HISTORIES OF EMISSION LINES IN A RAPIDLY IONIZING PLASMA

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ABSTRACT

The time histories of emission lines from successive ionization stages of impurity atoms in a plasma are predicted by solving the coupled rate equations governing the populations of these ionization stages with the help of a computer program. A detailed description of the program is given. An application of such predictions for the measurement of ionization rate coefficients of ions occuring in a rapidly ionizing plasma is discussed.

I. INTRODUCTION

Knowledge of the lifetime of various ionic stages of impurity atoms in high temperature hydrogen or deuterium plasmas is very important in controlled nuclear fusion research for the estimation of energy losses as well as in understanding, e.g., the physics of the solar corona (flares, etc.). The basic processes governing the ionic lifetimes are collisional ionization and the various recombination processes--radiative, dielectronic, three-body, whose relative importance is determined by the plasma conditions. In order to understand the relative importance of these processes, the plasma conditions could be simulated and the time histories of emission lines from various ionization stages be predicted by a computer program. The purpose of this report is to describe in detail such a computer code.[1] It was used for example, to determine the ionization rate coefficients of various ions using a Θ-pinch plasma[2,3] with added impurities. The principles of such measurements are as described by Hinnov.[4]

In Section II the basic equations and the adopted procedure for their solution are described. In Section III the set up of the program is described. In Section IV the description and listing of the program is given. In Section V sample test data are set up such that analytical solutions can be obtained. A comparison with the computer solution checks the accuracy. In Appendix I plotting subroutines are listed. In Appendix II an application of this program for the determination of ionization rates is discussed using the data from an experiment[5] as an example.

II. BASIC EQUATIONS

The impurity ions in a transient plasma go successively through the various ionization stages, the degree of ionization lagging behind the corresponding quasistationary corona equilibrium.

The density N_k of ions (K is the nuclear charge) in the total plasma Volume V is determined by the following rate equation:

$$\frac{d\,(N_k V)}{dt} = VN_{k-1}\, NI_{k-1} - VN_k\, NI_k + VN_{k+1}\, N\alpha_{k+1} - VN_k\, N\alpha_k \tag{1}$$

where N is the electron density, I_k is the ionization rate coefficient and α_k the recombination rate coefficient. The plasma volume would change with time in a Θ-pinch plasma due to compression or expansion. This variation was accounted for in our experiments by the assumption that particle losses are negligible, which is found to be valid in the operation of our Θ-pinch with a reverse bias field.

$$\frac{d}{dt}\,(NV) = 0.$$

$$\frac{dV}{dt} = -\frac{V}{N}\frac{dN}{dt} \tag{2}$$

This also assumes small concentrations of impurity ions such that electron production by ionization is negligible. Hence using Eq. 2 in 1

$$\frac{dN_k}{dt} = N_{k-1}\, NI_{k-1} - N_k\, NI_k + N_{k+1}\, N\alpha_{k+1} - N_k N\alpha_k + \frac{1}{N}\frac{dN}{dt} N_k \tag{3}$$

However, for different plasma machines and plasma conditions Eq. (2) could be different which would make the last term in Eq. (3)

to be different. Hence the last term in Eq. (3) is called the source term which should be appropriately modeled.

These coupled rate equations are solved numerically with the measured electron density and temperature given as input.

The following formulae were used for the rate coefficients in Eq. (3):

Ionization: A choice can be made to use one of the following approximations.

1. Semiempirical formula due to Kunze[2] derived by fiting to the semiemperical predictions of Lotz.[6] It is referred to here as "S(k)-Lotz & Kunze"

$$S(K) = SA(K) \left[\left(\ell n \, \frac{40(kT)}{E_i} \right)^3 + 40 \right] \frac{kT^{\frac{1}{2}}}{E_i + 3kT} \, e^{-E_i/kT} \; cm^3/sec \tag{4}$$

$$SA(K) = 7.5 \times 10^{-8} \, \frac{\eta i}{E_i} \tag{5}$$

Here "ηi" is the number of electrons in the i^{th} subshell (e.g. for the $1s^2 2s^2 2p$ configuration η_i is 1 for 2p, 2 for $2s^2$ and 2 for $1s^2$ subshells, and the ionization rate of the ground state is a sum of all these contributions) and E_i is the corresponding ionization energy. Both kT and E_i are in e.v. The constant SA(K) is given as input.

A comparison to another semiemperical formula due to Hinnov[4] was found to yield the same results as Eq. (4).

2. Summers[7] described the procedure for calculating the ionization rate coefficients using the Exchange Collisional

and Impact Parameter (E.C.I.P.) method due to Burgess.[8] This procedure is adopted into our program and the ionization rate is referred to as S(K)- Burgess and Summers.

$$S(K) = A(K)\ X\ \text{(Burgess and Summers rate.)}\ \ cm^3/sec \qquad (6)$$

A(K) is a multiplicative value to change the rate if one wishes. It is given as input. Other input data needed to evaluate Eq. (6) is described in the Comments of Subroutine Main - R/W in Sec. IV.

Recombination: Three processes of recombination are considered. Generally, for a rapidly ionizing plasma recombination rates are negligible. However, one has to check this especially for higher ionization stages. The total recombination rate is referred to as Alpha(K).

1. Radiative recombination: RALPHA
   For the evaluation of RALPHA a formula due to Seaton[9] (Eq. 4.3.35 Ref. 10) was adopted.

$$\text{RALPHA}(R\alpha_k) = 5.20.10^{-14}\ Z(E/kT)^{1/2}\ (0.429 + 0.5\ \ell n\ \frac{E}{kT} + 0.469\ (kT/E)^{1/3}\ \ (cm^3 sec^{-1}) \qquad (7)$$

where 'Z' is the effective charge of the recombining ion K (giving K-1) and E is the ionization potential of the ion upon recombination. (i.e. K-1)

2. Dielectronic recombination: DALPHA

For the evaluation of DALPHA simple formulae due to Landini and Monsignori Fossi[11] are used.

For ions pertaining to H, He, Ne, K to Ni DALPHA ($D\alpha_k$) =

$$1.60 \times 10^{-10} (Z+1)^2 F(K)(kT)^{-3/2} W(K)^{-1/2} \exp\left[\frac{-0.9134W(K)}{kT}\right] \tag{8}$$

where Z is the charge of the recombining ion, W(K) is the first excitation energy in e.v for the recombining ion and F(K) could be taken as the number of electrons in the outer shell (F(k)=1 for H-like, 2 for He-like, 6 for Ne-like ...)

For ions pertaining to Li to F, Na to Ar, Cu to Kr DALPHA($D\alpha_k$) =

$$1.6 \times 10^{-10} (Z+1)^2 F(K)(kT)^{-3/2} \exp\left[-0.9134 \frac{(Z+2.3) \quad W(K)}{3.3 \text{ kT}}\right] \tag{8}$$

where Z+1 and W(K) are defined as in Eq. 8. F (K) values are taken from Ref. 7.

3. Three body recombination: BALPHA

For the evaluation of three body recombination a formula due to Griem[12] was used.

$$\text{BALPHA } (B\alpha_k) = 1.4 \times 10^{-31} N \; Z^{-6} \left(E_i / kT\right)^2 \exp\left[E_i \; / \; kT(n^1+1)^2\right] \tag{9}$$

where N is the electron density, Z the charge of the ion before recombination and n^1 the quantum number of the Collision limit[12] i.e. the level from which radiative decay is about as probable as collisional excitation to higher levels.

$$n^1 \approx 1.26 \times 10^2 Z^{14/17} N^{-2/17} (E_i/kT)^{-1/17} \exp\left[4 E_i/17(n^1)^3 kT\right] \tag{10}$$

A plot of n^1 is given in Ref. 9.

Having determined the time history of ionic populations, the time histories of their emission lines could be predicted. The emission coefficient of an optically thin allowed line, whose upper level is mostly populated by electron collisions from the ground state is given by

$$\epsilon = \frac{h\nu}{4\pi} N X N_k \quad \text{ergs} / \text{cm}^3 \text{ sr sec} \tag{11}$$

We assume excited state populations to be small so that N_k represents the ground-state population. Also X is the excitation rate coefficient. If N and X are constant, the time history of the line is identical to the time history of the ion. However, variations in N and X can be accounted for even though the absolute value of X is not known. The time dependence of X is accounted for by the effective Gaunt-factor approximation.

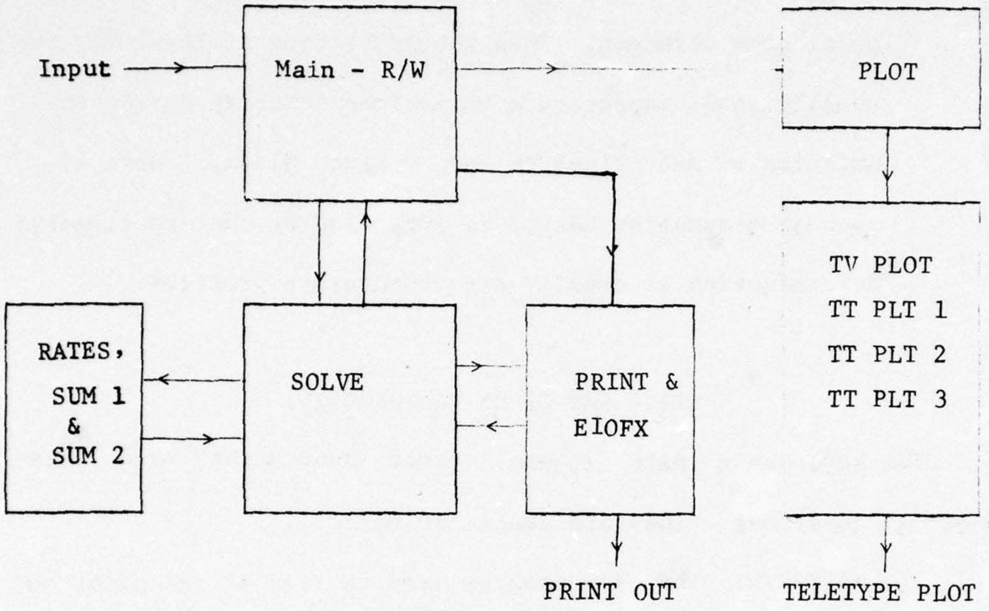
$$X = 1.6 \times 10^{-5} f e^{-\Delta E/kT} (\Delta E)^{-1} (kT)^{-1/2} \tag{12}$$

where ΔE is the excitation potential in ev and 'f' is the oscillator strength. This should be true at least for the usually small temperature variations occuring during the emission of many lines in our Θ-pinch plasma. However, such an assumption has to be supported by the experimental determination of density and temperature profiles.

III. SET UP OF THE PROGRAM

The code has a main program, four subroutines and three external functions. They are described below.

1. MAIN-R/W: The main program used to read in and print out the data, and control the rest of the program.
2. SOLVE: A subroutine that solves the differential equations.
3. RATES: A subroutine that interpolates density and temperature, calculates the rate coefficients and increments in populations at each fine time step 'J' required by SOLVE. External functions SUM1 and SUM2 are for the evaluation of S(K) - Burgess and Summers.
4. PRINT: Print is used to output the calculations of ionic populations calculated in "SOLVE". Print together with external function EIOFX calculate the intensities of spectral lines.
5. PLOT: The intensity as a function of time is stored for teletype plotting.



OUTPUT

The program TV PLOT and the Subroutines TT PLT 1, TT PLT 2, and TT PLT 3 are for teletype plotting the data stored by PLOT.

IV. PROGRAM DETAILS AND LISTING

The following variables are in the common block of each Subroutine.

J. Index counter counting the fine time steps in the Subroutine SOLVE. When J reaches Jmax the Subroutine PRINT is called and the output is printed. Then J is set back to 3.

Jmax: Given as data in Main-R/W. The maximum value J takes is Jmax.

ND: Number of ions ($\lesssim$ ION) for which SOLVE solves the differential equations. It is given as input.

H: Variable representing the step size (time) in SOLVE.

DTmax: Predicted value of H given as input.

Kstep: Counter counting the number of fine steps in the integration program SOLVE.

KSend: Maximum limit "Kstep" could take in the Subroutine SOLVE. It is given as input.

KDOB: Flag. If it becomes -1 the time step H is considered for doubling in SOLVE subroutine.

KHAV1
KHAV2
KHAV3 Flags used in SOLVE to decide whether at a certain time, the step size H is to be made half.

DOB1,
DOB2 Counters used in SOLVE to limit the maximum number of iterations in finding proper H.

T(60): Time at each fine time step J in SOLVE.

EPSI(60): Accumulated error indicating how well the integration is proceeding.

Y(60,18): Population density of each ionization stage at each time step.

YR(60,18): Increments in populations for each time step --i.e. $\frac{dNk}{dt}$. These are calculated in "RATES".

S(18): Ionization rate Coefficients.

Alpha(18): Total recombination rate Coefficients.

NTIME: Maximum number of coarse time steps for the input data.

TIME (100), DENS (100), TEMP (100): Electron density and temperature data at coarse time steps L=1 to NTIME given as input.

DNE(60), TE(60): Interpolated electron density and temperature data at each five time step J.

Ion: Maximum number of ions for which rate equations are going to be solved.

IonM1: Ion -1.

KION(18): Counter for the number of ions.

SA(18): The coefficients for the ionization rates calculated by the formula of Lotz and Kunze. They are given as input.

SB(18): Values used in Lotz and Kunze formula. (SB is set 3.)

SE(18): Ionization potentials for the ions given as input.

ANPRIM(18): Data for three body recombination in RATES to be given as input.

NAME(18): Identification of the plasma condition.

SFN(18): Oscillator strengths for the lines whose time histories are to be predicted.

SEX(18): Excitation potentials in eV for these lines.

ØØ1: Electron density divided by the sum of all ionic populations at t=0 μsecs.

YMIN: 10^{-4} times the sum of all ionic populations.

YYMIN: 10^{-6} times the sum of all ionic populations.

EN, ED, EH: Constants to check accuracy in SOLVE.

NDT, NAINI: Constants used in the program.

NA: A variable representing the stage of ionization below which populations are less than YMIN.

THI(60, 18): Theoretical intensities stored for plotting. Input data for dielectronic recombination (DALPHA) formulae due to Landini and Fossi.[11]

F(18): Given in Ref. 11.

W(18): First excitation energy in recombining ion. Given in Ref. 11.

Yes(18): A flag whose value is read in for each ion to decide which formula for DALPHA is to be used.

Flag: A flag decides whether experimental or theoretical intensities are to be plotted.

Tim: Variable used in "PRINT" to find the fine time steps that correspond to the Coarse time steps.

DIF 2: The difference between fine time step and the coarse time step evaluated in "PRINT".

TTT(60): The fine time steps that are equal to or close to the coarse time steps.

Flag 1: A flag read in input data which decides whether Burgess and Summers or Lotz and Kunze ionization rate coefficient is to be used.

M(I,K): Number of equivalent electrons in shell I of ion K.

H(I,K): Ionization energy in eV of an electron in shell "I" of ion "K". Five shells should be more than enough.

A(K): A factor multiplying Burgess and Summers ionization rate to match time histories.

PROGRAM DETAILS:

1. MAIN - R/W: It reads in the data and manages the rest of subroutines. The integer variables FLAG, FLAG1 and YES are flags whose

values given as input would make the required calculations. The possible manipulations are described in the comments of the listing of this subroutine. In the appendix II data is set up as an example. The array YI(J,K) is used to read in the experimental time histories. A brief description of the purpose of the following variables is given below.

A SUM: Sum of initial populations of all ions.

ØØ1: Electron density at time t=0 μs divided by A SUM. This is used in PRINT to normalize the calculated populations. This procedure is to check how the effect of compression was taken care of in the subroutine RATES by the variable ABL and how the smooth transfer of populations from one stage to the other is proceeding.

YMin and YYMin: These are used to avoid the accuracy check in SOLVE for ions with negligible populations at a certain time step J.

2. SOLVE: This subroutine solves the coupled differential equations by numerical integration using Adams predictor-corrector methods. A general outline of the working process of this subroutine is described below.

The flag NSTART takes values 1, 2 or 3 given as input data. If NSTART is set to 1, the program, between statement numbers 5 through 19, will try to find a proper time step H for continuing the solution with stability and convergence. An initial value for H (DTMAX) is given as input. Also the density and temperature information has to be given at one negative time (non physical) for this self starting procedure. This information is only useful for starting the program and does not influence the solution.

If NSTART is set to 2, the initial value for H given as input is used to continue the integration. However, the program tries to adjust "H" to obtain solutions within the accuracy requirements.

If NSTART is set to 3, the difference between coarse time steps 1 and 2 at which density and temperature information was given would be taken as the starting value of H and the program tries to adjust H, if required, to continue integration keeping the required accuracy.

The program had provisions to speed up the calculation by doubling the step size or to retrace back one time step and cut the step size to half and continue the integration within the accuracy requirements. The accuracy checks were done by using the values for EN, EH and ED as 1, .1 and .001 respectively. These values were found to yield good stability, convergence and accuracy in the running of SOLVE. In section V analytical solutions were compared with numerical solutions for a simple two ion system. Further details about the working of the program are in the comments of the listing of SOLVE.

3. RATES: It calculates the ionization and recombination rates, as well as increments in populations at each time step J. The variable ABL takes care of effects of any compression etc. The external functions SUM1 and SUM2 are used to calculate S(K)--Burgess and Summers if desired (i.e. Flag 1.GT.0). Other details are in comments of the listing.

PRINT: This subroutine prints the concentration of each ionization stage at each time step J. It calculates the intensities of emmission lines, using the external function EIOFX and prints them.

PLOT: The time histories of emission lines are written on a tape for later plotting.

MAIN - R/W

```
C
C  THIS PROGRAM IS FOR SOLVING COUPLED RATE EQUATIONS AND PREDICTING
C  TIME HISTORIES OF THE IMPURITY IONS AND THEIR EMISSON LINES IN A
C  RAPIDLY IONIZING PLASMA LIKE THAT OF A THETA PINCH.
C  DATA NEEDED AS INPUT IS ELECTRON DENSITY AND TEMPERATURE PROFILES
C  WITH RESPECT TO TIME AND THE CHARECTERISTIC DATA FOR EVALUATING
C  THE VARIOUS RATE COEFFICIENTS--IONZATION&RECOMBINATION(RADIATIVE,
C  THREE BODY&DIELECTRONIC) RATE COEFFICIENTS.
C
      INTEGER TIM,FLAG,FLAG1,YES
      DIMENSION YI(60,18)
      COMMON J,JMAX,ND,H,DTMAX,NDT,KSTEP,KSEND,END,ED,EH,EN,KDOB,
     1       KHAV1,KHAV2,KHAV3,DOB1,DOB2
      COMMON T(60),EPSI(60), Y(60,18),YR(60,18
     1       ),ANPRIM(18)
      COMMON S(18),ALPHA(18),DENS(100),TEMP(100),TIME(100),SA(18),SB(18)
     1       ,SE(18),NAME(8),KION(18),DNE(60),TE(60),SFN(18),SEX(18)
      COMMON  NTIME,ION,IONM1,NA,NAINI,001,YMIN,YYMIN
      COMMON TMI(60,18),TIM,FLAG,F(18),YES(18),W(18),M(5,18),HI(5,18)
     1 ,FLAG1,TTT(60),DIF2,A(18)
C
C  IN THIS PROGRAM COARSE TIME STEPS MEAN THE TIME STEPS AT WHICH
C  DENSITY AND TEMPERATURE INFORMATION IS GIVEN.
C
C  TIM   -IT IS A VARIABLE USED IN THE SUBROUTINE PRINT TO FIND THE
C          COARSE TIME STEPS AMONG THE FINE TIME STEPS GENERATED BY THE
C          SUBROUTINE SOLVE.
C
C  FLAG IS A FLAG TO INSTRUCT THE COMPUTER WHAT IS TO BE PLOTTED.
C   'FLAG' VALUES:
C      0 - EXPERIMENTAL INTENSITIES ONLY (PLOT THEM)
C      1 - BOTH THEORETICAL AND EXPERIMENTAL INTENSITIES (PLOT BOTH
C          OF THEM. (THE THEORETICAL INTENSITIES ARE THE ONES COMPUTED BY
C           THE SUBROUTINE SOLVE.) THIS VALUE CAN ONLY BE USED FOR
C           REMOTE TERMINAL PLOTTING BUT NOT FOR TELETYPE PLOTTING.
```

```
C              THIS IS THE WAY SUB ROUTINES TTSTORE & PLOTTER ARE CONSTRUC
C              -TED.
C         2 - THEORETICAL INTENSITIES ONLY  (PLOT THEM)
C
C  FLAG1 IS A FLAG TO INSTUCT THE COMPUTER WHICH FORMULAS FOR IONIZATION
C  ARE TO BE USED.
C  FLAG1 VALUES:
C              0 - SEMI EMPERICAL FORMULA DUE TO LOTZ&KUNZE IS USED.
C              1 - SEMI CLASSICAL FORMULAE DUE TO BURGESS&SUMMERS ARE
C                  USED.TWO SUBROUTINES SUM1&SUM2 DO THIS JOB.
C  EXPLANATION OF THE INPUT DATA FOR THE RATE COEFFICIENTS IS GIVEN
C  BELOW.
C   SA(K) &SB(K) ARE CONSTANTS USED IN LOTZ&KUNZE´S IONIZATION RATE
C   COEFFICIENT.IF FLAG1 IS NOT SET 0 THEN THESE ARE STILL READ BUT
C   NEVER USED.
C
C  THE FOLLOWING IS FOR SUMMERS&BURGESS IONIZATION RATE COEFFICIENT.
C   "M(I,K)"- NO OF EQUIVALENT ELECTRONS IN "I"SHELL OF ION K.
C   "H(I,K)"- IONIZATION ENERGY IN EV OF AN ELECTRON IN SHELL "I" OF ION
C   K. FIVE SHELLS SHOULD BE MORE THAN ENOUGH !
C
C  DALPHA IS DIELECTRONIC RECOMBINATION. THE FOLLOWING ARE NEEDED TO
C  IT´S EVALUATION.
C  ´F´ IS INPUT DATA FOR DALPHA.
C  ´W´ -FIRST EX ENERGY OF RECOMBINING ION- IN DALPHA.
C
      READ(5,100) (NAME(K),K=1,8)
  100 FORMAT(8A4)
    1 READ(5,101) ION,NTIME,NAINI,FLAG,FLAG1
  101 FORMAT(12I6)
      READ(5,102)(KION(K),SA(K),SB(K),SE(K),Y(2,K),ANPRIM(K),K=1,ION)
  102 FORMAT(I12,4E12.4,F12.4)
      READ(5,103) JMAX,ND,NDT,KSEND,END,ED,EH,   EN,DTMAX
  103 FORMAT(3I4,I8,5E8.1)
      READ(5,104) (TIME(K),TEMP(K),DENS(K),K=1,NTIME)
  104 FORMAT(3E12.4)
      READ(5,105) (SFN(K),SEX(K),K=1,ION)
  105 FORMAT(2F10.5)
```

```
      READ(5,106)(YES(K),F(K),W(K),K=1,ION)
  106 FORMAT(I3,F7.5,F10.5)
      IF (FLAG1.EQ.0) GO TO 107
      DO 129 K=1,ION
  129 READ(5,130)A(K),(M(I,K),HI(I,K),I=1,5)
  130 FORMAT (E10.4,(5(I2,F10.4)))
  107 IF (FLAG .GT. 1) GOTO 120
      NT=NTIME-2
      DO 110 J = 1,NT
      ITT(J)=TIME(J+2)
  110 READ(5,115) (YI(J,K),K=1,ION)
  115 FORMAT(13F4.2)
C
C  ALL THE NEEDED DATA IS READ BY NOW.IT WAS DONE IN THE FOLLOWING
C  ORDER. DATA FOR KUNZE&LOTZ,DENSITY &TEMP PROFILES,DATA FOR EXCITATION
C  ,DALPHA,SUMMERS&BURGESS,& EX PERIMENTAL TIME HISTORIES.
C
      DO 200 J=1,NT
  200 WRITE(6,116) (YI(J,K),K=1,ION)
  116 FORMAT(13F6.2)
C
C  NOW NORMALIZE AND PLOT THE EXPERIMENTAL INTENSITIES
C
      CALL PLOTT(YI,1,0)
      IF (FLAG .EQ. 0) STOP
C
C
C
  120 IONM1 = ION -1
      WRITE(6,200)
  200 FORMAT(1H1,10X,76H IONIZATION OF IMPURITY IONS IN A PLASMA WITH GI
     1VEN DENSITY AND TEMPERATURE ///)
  201 FORMAT(10X,10H IMPURITY ,8A4//)
      WRITE(6,201) (NAME(K),K = 1,8)
      WRITE(6,202) ION
  202 FORMAT(10X,24H NUMBER  OF  IONS  ION =I4//)
      IF (FLAG1.EQ.0)GO TO 211
      WRITE(6,212)
  312 FORMAT(10X,42H DATA FOR ECIP IONIZATION RATE COEFFICIENT //)
      DO 313 K=1,ION
  313 WRITE(6,314)(KION(K),(M(I,K),HI(I,K),I=1,5),Y(2,K),ANPRIM(K),A(K))
  314 FORMAT(5X,I2,5(I2,E10.4),E10.4,F3.1,F10.6)
      WRITE(6,315)
  315 FORMAT( ///10X,' THE IONIZATION RATE COEFFICIENTS ARE CALCULATED
     1BY THE FORMULA'//10X,'S = A * SEMICLASSICAL RATE COEFFICIENT '
     2///10X, ' THE FORMULA USED FOR TOTAL RECOMBINATION:'//
     3  10X, 89H ALPHA = 5.2E-14*Z*SQRT(E(I-1)/T) * (0.429 + 0.5*LN(E(I-
     41)/T) + 0.469*CBRT(T/E(I-1))  +  /15X,75H1.4E-31 * N * (NPRIME/Z)*
     5*6 * (E(I-1)/T)**2 * EXP(E(I-1)/(T*(NPRIME+1)**2)),2H +,/15X ,
     6' DIELECTRONIC RECOMBINATION(LANDINI&FOSSI SOLAR PHYSICS 20,322P
     7 (1971))'///
     811X,'FOR THE EXCITATION WE USE G(EFF) APPROXIMATION'//10X,' X= 1.5
     98E-05*FN*P*(EXP-EX/T)/(EX*SQRT(T))'////)
      GO TO 316
  211 WRITE(6,203)
  203 FORMAT(10X,' CHARACTERISTIC DATA FOR THE IONS '//15X,
     1   4H ION,5X,2H A,10X,2H B,10X7H E (EV),10X,'INITIAL DENSITY',15X,
     2   6HNPRIME//)
      WRITE(6,204) (KION(L),SA(L),SB(L),SE(L),Y(2,L),ANPRIM(L),L=1,ION)
  204 FORMAT(15X,I3,1X,3E12.4,12X,E12.4,10X,F12.4)
      WRITE(6,205)
  205 FORMAT( ///10X,' THE IONIZATION RATE COEFFICIENTS ARE CALCULATED
     1BY THE FORMULA'//10X, ' S = A*((LN(40*T/E)**3)+40)*SQRT(T)*EXP(-E
     2/T)/(E+BT)'///10X, ' THE FORMULA USED FOR TOTAL RECOMBINATION:'//
     3  10X, 89H ALPHA = 5.2E-14*Z*SQRT(E(I-1)/T) * (0.429 + 0.5*LN(E(I-
     41)/T) + 0.469*CBRT(T/E(I-1))  +  /15X,75H1.4E-31 * N * (NPRIME/Z)*
     5*6 * (E(I-1)/T)**2 * EXP(E(I-1)/(T*(NPRIME+1)**2)),2H +,/15X ,
     6' DIELECTRONIC RECOMBINATION(LANDINI&FOSSI-SOLAR PHY.20(1971))'///
     711X,'FOR THE EXCITATION WE USE G(EFF) APPROXIMATION'//10X,' X= 1.5
     88E-05*FN*P*(EXP-EX/T)/(EX*SQRT(T))'////)
  316 WRITE(6,208) JMAX,ND,NDT,KSEND,END,ED,EH,EN,DTMAX
  208 FORMAT(10X,'CONSTANTS FOR THE INTEGRATION PROGRAM '//
     1   10X,7H JMAX =I4,5X,5X,5H ND =I4,5X,6H NDT =I4,
     25X,8H KSEND =I8//10X,6H END =E8.1,5X,5H ED =E8.1,5X,5H EH =E8.1,
     3   5X,5H EN =E8.1,5X,9H DTMAX =E8.4//)
      WRITE(6,214)
  214 FORMAT(///10X,36H DATA FOR DIELECTRONIC RECOMBINATION//,
     *15X,3HION,3X,7HFORMULA,3X,7H F.OR.N,8X,6H W(EV)//)
      WRITE(6,215)(KION(K),YES(K),F(K),W(K),K=1,ION)
  215 FORMAT(15X,I3,7X,I3,7X,F3.0,2X,F10.5)
      WRITE(6,206)
  206 FORMAT(1H1,10X,'INPUT DENSITY & TEMPERATURE PROFILES ARE:'///
     1   15X,5H TIME,3X,11H TEMP (EV) ,16H DENSITY(CM**-3)//)
      WRITE(6,207) (TIME(K),TEMP(K),DENS(K),K=1,NTIME)
  207  FORMAT( 10X,3E12.4)
      WRITE(6,212)
  212 FORMAT(//10X,' DATA FOR THE EXCITATION OF THE IONS '//15X,4H ION
     1,5X,3H FN,8X,6HEX(EV)//)
      WRITE(6,213) (KION(K),SFN(K),SEX(K),K=1,ION)
  213 FORMAT(15X,I3,1X,F12.5,1X,F12.3)
      WRITE(6,210)
  210 FORMAT(1H1)
C
C
         ASUM = 0.0
         DO 301 K = 1,ION
  301    ASUM = ASUM + Y(2,K)
         001 = DENS(2)/ASUM
         YMIN = 1.0E-04*ASUM
         YYMIN = 1.0E-06*ASUM
         T(2) = 0.0
         NA = NAINI
         TIM = 3
         CALL SOLVE(1,NEND)
         CALL PRINT
         WRITE(6,209) NEND
  209 FORMAT(1H0,50X,7H NEND =I5//10X, 'HURRAY!!!!!!SUCCESSFUL RUN !!!')
         IF(NEND.GT.1) GO TO 500
C
C THE FOLLOWING PART IS FOR PLOTTING:
C
      DO 370 K=1,ION
      DO 360 I=3,NTIME
  360 THI(I-2,K)=THI(I,K)
  370 CONTINUE
      DO 371 I=3,NTIME
  371 TTT(I-2)=TTT(I)
      NTT=NTIME-2
      DO 372 K=1,ION
      DO 373 I=1,NTT
      WRITE(6,350) TTT(I),THI(I,K),K
  350 FORMAT(10X,'TTT=',E12.4,5X,'THI(I,K)=',E12.4,5X,'K=',I3/)
  373 CONTINUE
  372 CONTINUE
C  IN ABOVE  WHAT WAS DONE IS THAT 'TTT(I) & THI(I) ' ARE MADE TO START
C  FROM I=1. ORIGINALLY I(TIM) WAS SET=3 TO AVOID THE FIRST TWO COARSE
C  TIME STEPS
C  NOW NORMALIZE AND PLOT THE THEORETICAL INTENSITIES STORED IN 'THI'
C
      IF (FLAG1.EQ.0) GO TO 400
      CALL PLOTT(THI,2,1)
      GO TO 500
  400 CALL PLOTT(THI,2,2)
C
C  THE CALCULATIONS & PLOTTING ARE OVER .
C
  500 STOP
      END
      SUBROUTINE SOLVE(NSTART,NEND)
C
C INTEGPATION PROGRAM FOR THE COUPLED 1-ORDER DIFFERENTIAL EQUATIONS
C NUMERICAL INTEGRATION DONE BY " PREDICTOR CORRECTOR " METHODS OF ADA
C MS & MOULTON TYPE. THIS PROGRAM HAS THE OPTION FOR SELF STARTING. IT
C VARIES THE STEP SIZE-H TO OBTAIN THE REQUIRED ACCURACY.
C
      COMMON J,JMAX,ND,H,DTMAX,NDT,KSTEP,KSEND,END,ED,EH,EN,KDOB,
     1          KHAV1,KHAV2,KHAV3,DOB1,DOB2
      COMMON T(60),EPSI(60), Y(60,18),YR(60,18
     1          ),ANPRIM(18)
      COMMON S(18),ALPHA(18),DENS(100),TEMP(100),TIME(100),SA(18),SB(18)
     1          ,SE(18),NAME(8),KION(18),DNE(60),TE(60),SFN(18),SEX(18)
      COMMON  NTIME,ION,IONM1,NA,NAINI,001,YMIN,YYMIN
      COMMON THI(60,18),TIM,FLAG,F(18),YES(18),W(18),M(5,18),HI(5,18)
     !  ,FLAG1,TTT(60),DIF2,A(18)
C
      INTEGER DOB1,DOB2,MXDOB
      INTEGER END
C
C COEFFICIENTS FOR THE PREDICTOR CORRECTOR FORMULAE.
C
        MXDOB=2**25
        CF1 = 2./3.
        CF2 = 4./3.
        CF3 = 1./8.
        CF4 = 1./12.
        CF5 = 5./12.
        CF6 =23./12.
        CF7 = 1./24.
        CF8 = 5./24.
        CF9 = 9./24.
        CF10= 19./24.
        NSTART = NSTART
    2   GO TO (5,6,4),NSTART
```

```
C
C   SET THE VALUES AT THE THREE INITIAL POINTS.
C
  4     H=T(2)-T(1)
      IF(H) 101,100,101
 100    NEND=6
      WRITE(6,600)
 600  FORMAT(1X,' EXIT DUE TO TIMESTEP H AT #4 OR #101 ')
      RETURN
 101  IF(ABS(T(3)-T(2)-H)-ABS(H)*.01)102,102,100
 102    N1=NDT
      Z1=ABS(H)
        NDT=0
 105  IF(Z1-ABS(DTMAX))103,104,104
 103    NDT=NDT+1
        Z1=Z1*2.
        GO TO 105
 104 DOB1=MXDOB/2**NDT
        NDT=N1
        J = 1
      CALL RATES
        J=2
      CALL RATES
        J = 3
      CALL RATES
        EPSI(2) = 0.
        KSTEP = 3
        GO TO 3
C
C PROGRAM STARTS HERE IF NTART=1.
C
  5     H = DTMAX * 2. **(-NDT)
        DOB1 = MXDOB/2**NDT
        J = 2
C
C INITIALIZE
C
      CALL RATES
```

```
        DO 13  N = NA,ND
        Y (1,N) = Y (2,N)
        YR(1,N) = YR(2,N)
        Y (3,N) = Y (2,N)
   13   YR(3,N) = YR(2,N)
C
C ITERATION OF THE ADAMS MOULTON K=2 CORRECTOR.IT DOES 5 ITERATIONS HERE
C IF THE CONVERGENCE IS NOT FAST ENOUGH TO MEET THE ACCURACY CHECK, ITCU
C TS THE TIMESTEP BY HALF AND TRIES AGAIN FOR FIVE ITERATIONS. THIS GOES
C ON UNTIL DOB1 BECOMES ZERO THAT IS NDT TIMES.
C
C
   12   T(1) = T(2) - H
        T(3) = T(2) + H
        IT1  = 0
        IT2  =-1
   24   ZE  = 0.
        Z1 = EN * H
        DO 18 N = NA,ND
        Z2 = CF1 * YR(2,N)
        Y(1,N ) = Y(2,N) - (CF5 * YR(1,N) + Z2 - CF4 * YR(3,N)) * H
        ZY =     Y(2,N) + (CF5 * YR(3,N) + Z2 - CF4 * YR(1,N)) * H
C
C THIS  "IF" OMITS THE ACCURACY CHECK FOR SMALL Y(J,N), (E.G. ZERO)
C
            IF( Y(1,N) - YYMIN) 18,18,220
  220   Z2 = ABS(ZY - Y(3,N))/(ABS(Y(2,N)) + (ABS(YR(1,N))+ABS(YR
     1  (2,N)) + ABS(YR(3,N)))* Z1)
        ZE = AMAX1(ZE,Z2)
   18   Y(3,N ) = ZY
      IF (IT2) 19,20,20
C
C THE FOLLOWING 'IF' IS ACCURACY CHECK.
C
   20   IF(ZE - EH/16.) 21,21,22
  601 FORMAT(1X,'ZE=',F10.5/)
   22   IT1 = IT1 + 1
      WRITE(6,601) ZE
```

```
         IF(IT1 - 5) 19,23,23
   19    J = 1
      CALL RATES
         J = 3
      CALL RATES
         IT2 = 1
         GO TO 24
   23 DOB1=DOB1/2
         H = 0.5 * H
      WRITE (6,602)
  602 FORMAT(1X,'ITERATION DID NOT SUCCEED.SO TRY HALF THE TIME STEP'
     1 /)
      IF (DOB1.NE.0) GO TO 12
   25    NEND = 3
      WRITE(6,700)
  700 FORMAT(1X,///' EXIT AT #25-SOLVE.INPUT HMAX IS TOO LARGE ')
         RETURN
  603 FORMAT(1X,'BY NOW IT GOT HOLD OF THREE POINTS'/)
C
C TRY THE NEXT POINT--T(4).
C *******************     *******      ********
   21    KSTEP = 1
      WRITE(6,601) ZE
      WRITE(6,603)
      DOB2=DOB1
         J = 3
    3    EPSI(3)=0.
         KDOB=1
         KPRINT = 1
         KHAV1 = 1
         KHAV2 = 1
C
C NORMALCASE OF INTEGRATION.
C
  604 FORMAT(1X,' NORMAL CASE ')
    6    IF(KHAV1) 33,34,34
   33    IF(KHAV3) 35,29,29
   29    KHAV1 = 1
```

```
      KHAV2 = 1
    WRITE(6,604)
      GO TO 34
  35  KHAV3 = KHAV3 + 1
  34  IF(J -JMAX) 36,37,37
C
C RESET PRINT
C
  37  IF(KPRINT) 26,27,27
  27 CALL PRINT
  26  KPRINT = 1
      J1 = JMAX - 2
      NJ = 1
      DO 38 J = J1,JMAX
      T(NJ) = T(J)
      EPSI(NJ) = EPSI(J)
      DO 43 N = NA,ND
      Y(NJ,N) = Y(J,N)
  43  YR(NJ,N) = YR(J,N)
  38  NJ = NJ + 1
      J = 3
C
C EXTRAPOLATION: PREDICT AT THE NEXT TIME STEP WITH ADAMS K=2 PREDICTOR
C
C     EXTRAPOLATION
C
  36  T(J + 1) = T(J) + H
    WRITE(6,605)
 605 FORMAT(1X,' NORMALCASE. EXTRAPOLATION.')
      IF (H-DTMAX)47,48,48
  47 DOB2=DOB2+DOB1
  48  DO 55 N = NA,ND
  55  Y(J+1,N) = Y(J,N) + (CF5*YR(J-2,N)-CF2*YR(J-1,N)+CF6*YR(J,N))*H
      J = J + 1
    CALL RATES
C
C INTERPOLATION : CORRECTION WITH ADAMS K=3 CORRECTOR.
C
```

```
          ZE = 0.0
       WRITE(6,606)
  606 FORMAT(1X,' INTERPOLATION.')
          Z1 = EN * H
          DO 61 N = NA,ND
          ZY = Y(J-1,N)+(CF7*YR(J-3,N)-CF8*YR(J-2,N)+CF10*YR(J-1,N)+CF9*
     1    YR(J,N))*H
C THIS 'IF' OMITS THE ACCURACY CHECK FOR SMALL Y  ( E.G. ZERO)
                IF(Y(J,N) - YYMIN) 61,61,211
  211     Z2 = ABS(ZY-Y(J,N))/(ABS(ZY)+(ABS(YR(J,N))+ABS(YR(J-1,N))+
     1    ABS(YR(J-2,N))+ABS(YR(J-3,N))) * Z1)
          ZE = AMAX1(ZE,Z2)
   61     Y(J,N) = ZY
          EPSI(J) = 0.5 * EPSI(J-1) + ZE
          KSTEP = KSTEP + 1
       WRITE(6,607)KSTEP,END,J,EPSI(J)
  607 FORMAT(1X,' KSTEP= ',I5,'END',F10.5,'J',I5,'EPSI',F10.5/)
          IF (KSTEP - KSEND) 62, 63, 63
   63     NEND = 2
       WRITE(6,710)
  710 FORMAT(1X,///' NUMBER OF STEPS (KSTEP) BECAME GT THAN LIMIT
     1 KSEND')
          RETURN
   62     IF (END)            64,56 ,56
   64     NEND = 1
          RETURN
   56     IF (KSTEP-4) 49,40,40
   49     IF (EPSI(J) - EH/8.) 6,6,23
C
C CONTINUE INTEGRATION *********************
C
   40     IF (H - DTMAX)      67, 70, 70
   67     IF (KDOB)           68, 69, 69
   69     KDOB = KDOB - 1
          GO TO 70
C
C #71-TO-#79 BELOW ARE FOR DOUBLING THE STEP SIZE. #6-TO-#49 IN ABOVE
C FOR STEP SIZE KEPT SAME. #80-TO-#95 ARE TO CUT THE STEP SIZE BY HALF.
```

```
C
  68    IF (EFSI(J) - ED)  71, 70, 70
  71 Z=DOB1.AND.DOB2
C
C .AND. IS A MANIPULATIVE OPERATOR. Z IS ZERO AS DOB1 IS NOT=DOB2(#47)
C
        IF (Z)               6 , 72, 6
  72    NJ = J
        IF (J - 4)           73, 73, 74
  73    J = JMAX - 1
        KPRINT = -1
        GO TO 28
  74    J = J - 2
  28    T(J - 1) = T( J )
        T( J)    = T( NJ )
        EPSI(J-1) = EPSI(J)
        EPSI(J)   = EPSI(NJ)
        DO 79 N = NA,ND
        Y (J-1,N) = Y (J,N)
        Y(J,N)   = Y (NJ,N)
        YR(J-1,N) = YR(J,N)
  79    YR(J,N)   = YR(NJ,N)
     DOB1=DOB1*2
        H = 2.*H
        KDOB = 1
        KSTEP = KSTEP-2
        GO TO 6
C
C HALF THE TIME STEP.
C
  70    IF (EFSI(J)-EH) 6,6,80
  80    IF (KMAV2) 81,82,82
  81    NEND = 5
     WRITE(6,730)
 730 FORMAT(1X,///' THE ACCUMALATED ERROR IS GT THAN EH EVEN IN THE
    1 RECALCULATION OF TWO EARLIER TIME STEPS ! ')
        RETURN
  82    IF (KMAV1) 83,83,84
```

```
   84    KHAV1 = -1
         KHAV3 = -2
      DOB2=DOB2-DOB1
      DOB1=DOB1/2
         H = 0.5 * H
      IF(DOB1.NE.0) GO TO 86
   85    NEND = 4
      WRITE(6,740)
  740 FORMAT(1X,///' EXIT AT #85 AS DOB1 BECAME ZERO.I.E TOO MANY ITERAT
     1IONS.INPUT HMAX IS TOO LARGE. ')
         RETURN
   83    KHAV2 = -1
      DOB2=DOB2-DOB1*3
         KSTEP = KSTEP-2
         IF (KSTEP-2) 96,96,30
   96    KSTEP = 4
   30    J = J - 2
         IF(J-2) 31,31,86
   31    J = JMAX - 1
         KPRINT = -1
C
   86    T(J) = T(J - 1)
         EPSI(J) = EPSI(J - 1)
         DO 32 N = NA,ND
         Y (J,N) = Y (J -1,N)
   32    YR(J,N) = YR(J -1,N)
         T(J - 1) = T(J) - H
         EPSI(J - 1) = EH
         Z = 0.5 * H
      DO 95 N=NA,ND
   95    Y(J - 1,N) = (Y(J,N)+Y(J-2,N)-(YR(J,N)-YR(J-2,N))*Z)*0.5
         J = J - 1
      CALL RATES
         J = J + 1
         GO TO 6
      END
      SUBROUTINE RATES
C
C RATE COEFFICIENTS AND INCREMENTS IN POPULATIONS YR(J,K) AT EACH TIME
C STEP J ARE CALCULATED.
C
      INTEGER YES,FLAG1
      COMMON J,JMAX,ND,H,DTMAX,NDT,KSTEP,KSEND,END,ED,EH,EN,KDOB,
     1        KHAV1,KHAV2,KHAV3,DOB1,DOB2
      COMMON T(60),EPSI(60),Y(60,18),YR(60,18
     1        ),ANPRIM(18)
      COMMON S(18),ALPHA(18),DENS(100),TEMP(100),TIME(100),SA(18),SB(18)
     1        ,SE(18),NAME(8),KION(18),DNE(60),TE(60),SFN(18),SEX(18)
      COMMON  NTIME,ION,IONM1,NA,NAINI,001,YMIN,YYMIN
      COMMON THI(60,18),TIM,FLAG,F(18),YES(18),W(18),M(5,18),HI(5,18)
     !    ,FLAG1,TTT(60),DIF2,A(18)
C
      IF( T(J) + DTMAX - TIME(NTIME)) 6,7,7
    7    END = -1.0
C
C INTERPOLATION OF DENSITY AND TEMPERATURE
C
    6 DO 1 L = 1,NTIME
      IF( T(J)-TIME(L) ) 3,2,1
    1 CONTINUE
    2    DNE(J) = DENS(L)
         TE(J) = TEMP(L)
         ABL = ( DENS(L+1)-DENS(L-1))/((TIME(L+1)-TIME(L-1))*DENS(L))
      GO TO 4
    3    DT = TIME(L)- TIME(L-1)
         RDT = (T(J)-TIME(L-1))/DT
         DIFFD = DENS(L)- DENS(L-1)
         DNE(J) = DENS(L-1) + DIFFD*RDT
         TE(J) = TEMP(L-1) + ( TEMP(L) - TEMP(L-1))*RDT
         ABL = DIFFD/(DT*DNE(J))
C
```

```
C CALCULATION OF IONIZATION&RECOMBINATION RATE COEFFICIENTS.
C
        XSE = 0.0
        XNPRIM = 0.0
    4   DO 25 K = NA,ION
        IF (FLAG1.EQ.0)GO TO 26
C
C   FLAG1 # 0 . EVALUATE &USE ECIP IONIZATION RATE - BURGESS&SUMMERS.
C
        S(K)=COEF(K,TE(J),M(1,K),HI(1,K),M(2,K),HI(2,K),M(3,K),HI(3,K),
      1M(4,K),HI(4,K),M(5,K),HI(5,K))*A(K)
        GOTO 30
   26   AAA = 40.0 * TE(J) / SE(K)
        IF(AAA-1.0) 20,20,21
     20 AAA = 1.0
C
C   FLAG1=0.EVALUATE & USE SEMIEMPERICAL IONIZATION RATE - LOTZ&KUNZE.
C
     21     S(K) = SA(K)*((ALOG(   AAA           )**3) + 40.0)*SQRT(TE(J))*E
       1    XP(-SE(K)/TE(J))/(SE(K) + SB(K)*TE(J))
   30   IF(XSE) 9,9,10
     10 IF(XNPRIM) 12,12,11
C
C   EVALUATE THREEBODY RECOMBINATION "BALPHA" -DUCHS&GRIEM,PHYS.FLUIDS
C   (1966)VOL 9.
C
     11 BBB = XSE/(TE(J)*(XNPRIM+1.0)*(XNPRIM+1.0))
        IF(BBB-25.0) 19,19,18
     18 BBB = 25.0
     19 BALPHA = 1.4E-31*DNE(J)*((XNPRIM/(FLOAT(K)-1.0))**6) * ((XSE/TE(J)
      1   )**2)* EXP(BBB)
        GO TO 13
     12 BALPHA = 0.0
C
C NOW EVALUATE DIELECTRONIC RECOMBINATION ´DALPHA´ -LANDINI&FOSSI.
C
        IF(YES(K).EQ.1)GO TO 14
C
```

```
C   YES=1 MEANS ION IS H,HE,NE,K-NI LIKE ION (RECOMBINING)
C
      GO TO 15
  14  DALPHA=1.60E-10*((FLOAT(K))**2)*F(K)*SQRT(W(K))*EXP(-0.9134*
     :W(K)/TE(J))/SQRT(TE(J)**3)
C
C IN 14 F(K) IS NO OF ELECTRONS IN THE OUTER SHELL.K IS ION.EG.CV.
C
      GO TO 13
C
C IF YES#1 RECCMBINING ION IS LI-F,NA-AR LIKE ION.F(K)IS GIVEN BY
C LONDINI&FOSSI PAPER TABLE 2.
C
  15  DALPHA=1.60E-10*((FLOAT(K))**2)*F(K)*EXP(-0.9134*(FLOAT(K)+1.3)*W
     :(K)/(3.3*TE(J)))/SQRT(TE(J)**3)
C
C   EVALUATE RADIATIVE RECOMBINATION "RALPHA"
C
C
  13  RALPHA=5.20E-14*(FLOAT(K)-1.0)*SQRT(XSE/TE(J))*(0.429+
     1 0.5 *ALOG(XSE/TE(J))+0.469*CBRT(TE(J)/XSE))
      ALPHA(K)=BALPHA+DALPHA+RALPHA
      GO TO 5
   9  ALPHA(K)=0.0
   5  XNPRIM=ANPRIM(K)
      WRITE(6,17)K,TE(J),BALPHA,DALPHA,RALPHA,ALPHA(K),S(K)
  17  FORMAT(10X,I2,6E10.4)
   25    XSE = SE(K)
C
C   TEST FOR NEGATIVE DENSITIES.
C
      DO 50 K = NA,ION
         IF ( Y(J,K)) 51,50,50
   51            Y(J,K) = 0.0
   50 CONTINUE
C
C  INCREMENTS IN POPULATIONS FOR USE IN SOLVE..-PREDICTOR
C   -CORRECTOR METHOD OF SOLVING.
```

```
C
      IF(NA-1) 70,70,71
   70   YR(J,1)=-DNE(J)*(Y(J,1)*S(1)-Y(J,2)*ALPHA(2))+ABL*Y(J,1)
      NAA = 2
      GO TO 72
   71 NAA = NA
      ALPHA(NA)=0.0
      S(NA - 1) = 0.0
   72 DO 8 K = NAA,IONM1
        YR(J,K)=DNE(J)*(Y(J,K-1)*S(K-1)+Y(J,K+1)*ALPHA(K+1)
     1           -Y(J,K)*(S(K)+ALPHA(K))) + ABL*Y(J,K)
    8   CONTINUE
        K = ION
        YR(J,K)=DNE(J)*(Y(J,K-1)*S(K-1)-Y(J,K)*ALPHA(K)) + ABL*Y(J,K)
      RETURN
      END
```

SUM1

```
C
C  THIS IS EVALUATION OF E.C.I.P IONIZATION RATE COEFFICIENT USING
C  SEMI-CLASSICAL THEORY OF A.BURGESS.
C
C  THE FOLLOWING IS COMPUTER FORTRAN TRANSLATION DONE BY M.BLAHA
C  OF THE CALCLLATION PROCEDURE DESCRIBED BY SUMMERS IN THE APPELTON
C  LABORATORY REPORT I.M.367 (1974) PAGES 5&6.
C  INCORPORATICN OF THIS PROGRAM IN TO THE CODE FOR RAPIDLY IONIZING
C  PLASMAS WAS DONE BY RAJU DATLA.
C
      FUNCTION COEF(K,TT,I ,CHI1,J ,CHI2,L ,CHI3,
     1   M ,CHI4,NA,CHI5)
      DIMENSION X(10),OM(10),TEMP(10),N(5),CHI(5)
C
C  "X"&"OM" ARE "X(K)"&"OMEGA(K)" IN PAGE 5.THEY ARE THE NODES AND
C  WEIGHTS OF AN N-POINT GAUSS-LAGUERRE QUADRATURE.
C  "N(I) & CHI(I)" ARE NO OF EQUIVALENT ELECTRONS IN "I" SHELL&
C  IONIZATION ENERGY OF AN ELECTRON IN THAT SHELL.
C
      DATA X/0.137793,0.729455,1.808343,3.401434,5.552496,8.330153,
     1   11.843786,16.279258,21.996586,29.920697/, OM/0.308441,
     2   0.401120,0.218068,0.620875E-01,0.950152E-02,0.753008E-03,
     3   0.282592E-04,0.424931E-06,0.183956E-08,0.991183E-12/
C
C
      Z=K
C
C
      N(1)=I
      N(2)=J
      N(3)=L
      N(4)=M
      N(5)=NA
      CHI(1)=CHI1
      CHI(2)=CHI2
      CHI(3)=CHI3
      CHI(4)=CHI4
      CHI(5)=CHI5
      DO 7 I=1,5
      IF (N(I).EQ.0) GO TO 7
      CHI(I)=CHI(I)/13.606
    7 CONTINUE
      IT=1
      TEMP(1)=TT
      COEF=0.0
      DO 11 NE=1,5
      IF (N(NE).EQ.0) GO TO 11
      SUM=0.0
      AN=Z/SQRT(CHI(NE))
C
C  "AN" IS "NU" IN PAGE 6.
C
      DO 12 K=1,10
      EPS=TEMP(IT)*X(K)/13.606+CHI(NE)
C
C  2EPS" IS SYMBOL EPSILON IN PAGE 5.
C
      B=(EPS-CHI(NE))/CHI(NE)
      C1=B-(B+1)*ALOG(B+1)/(B+2)
      C2=1.0-1.0/(B+1)**3
      Q=C1/(B+2)+0.65343*C2*YP(Z,AN,B)/AN
C
C  "YP" IS THE FUNCTION Y(DELTA) IN PAGE 6.THIS IS EVALUATED IN SUM2
C  AS A SEPARATE FUNCTION.
C
      Q=4*Q/((E+1)*CHI(NE)**2)
      SUM=SUM+EPS*Q*OM(K)
   12 CONTINUE
      A=13.606*CHI(NE)/TEMP(IT)
      COEF=COEF+N(NE)*SUM*EXP(-A)
   11 CONTINUE
      COEF=21.7203E-09*COEF*SQRT(13.606/TEMP(IT))
C
```

```
C  IN C.G.S (2*ALPHA*C/SQRT(PI))*PI*(A**2)=21.7203E-09
C
         RETURN
         END
```

SUM2

```
C
C   "YP" IS A FUNCTION REFERENCED IN COEF. SO
C  E.C.I.P IONIZATION RATE COEFFICIENT EVALUATION CONTINUED.
C
      FUNCTION YP(Z,AN,B)
      DIMENSION AA(20),BB(20)
C
C  THE FOLLOWING IS DATA FOR AA&BB WHICH ARE A(J) & B(J) IN PAGE 6
C  AND TABLE 19.
C
      DATA AA/2.3916,1.6742,1.2583,0.9738,0.7656,0.6078,0.48561,0.38976,
     1   0.31388,0.25342,0.20501,0.16610,0.13476,0.10944,0.08896,
     2   0.07237,0.058903,.047971,0.039086,0.031860/,BB/1.0091,
     4   0.3015,0.1314,0.0763,0.0504,0.03561,0.02634,0.01997,0.01542,
     5   0.01205,0.950E-02,0.757E-02,0.602E-02,0.484E-02,0.389E-02,
     6   0.3123E-02,0.2535E-02,0.2047E-02,0.1659E-02,0.1344E-02/
      A=SQRT(B+1.0)
      D=(Z/AN)*((5*AN**2+1)/(4*Z)+2*AN**2*A/(Z*Z*(B+2)))/(A+SQRT(B))
C
C  "D" IS "DELTA" IN PAGE 6.
C
      IF (D.LE.0.1) GO TO 1
      IF (D.GE.2.0) GO TO 2
      I=10*D
      R=10*D-I
      S=I+1-10*D
      YP=R*AA(I+1)+S*AA(I)+((R**3-R)*BB(I+1)+(S**3-S)*BB(I))/6.0
      RETURN
    1 A=ALOG(1.1229/D)
      YP=A+0.25*D*D*(1.0-2*A*A)
      RETURN
    2 YP=1.5707963*EXP(-2*D)*(1.0+0.25/D-0.09375/D**2+0.0703125/D**3
     1   -0.0472/D**4)
      RETURN
      END
      SUBROUTINE PRINT
C
C SUBROUTINE TC PRINT THE THEORICAL INTENSITIES AND IONIC POPULATIONS
C  COMPUTED BY 'SOLVE'.
C
      INTEGER TIM
      COMMON J,JMAX,ND,H,DTMAX,NDT,KSTEP,KSEND,END,ED,EH,EN,KDOB,
     1          KHAV1,KHAV2,KHAV3,DOB1,DOB2
      COMMON T(60),EPSI(60), Y(60,18),YR(60,18
     1          ),ANPRIM(18)
      COMMON S(18),ALPHA(18),DENS(100),TEMP(100),TIME(100),SA(18),SB(18)
     1          ,SE(18),NAME(8),KION(18),DNE(60),TE(60),SFN(18),SEX(18)
      COMMON  NTIME,ION,IONM1,NA,NAINI,001,YMIN,YYMIN
      COMMON THI(60,18),TIM,FLAG,F(18),YES(18),W(18),M(5,18),HI(5,18)
     !    ,FLAG1,TTT(60),DIF2,A(18)
      DIMENSION CONC(18),XINT(18),ATOTAL(100)
C
      IF( ION - 9) 1,1,2
C
    1 WRITE(6,201) (KION(L),L=1,9)
  200 FORMAT(E12.4,9F11.4,F10.4,3X,I2)
  201 FORMAT(1H1,12H  TIME (SEC),4X,5H ION I2,4X,5H ION I2,4X,5H ION I2,
     1    4X,5H ION I2,4X,5H ION I2,4X,5H ION I2,4X,5H ION I2,4X,5H ION I
     22,4X,5H ION I2,4X,3HSUM,5X,2HNA///)
  301 FORMAT(1H1,12H  TIME (SEC),8X,5H INT I2,5X,5H INT I2,5X,5H INT I2,
     1    5X,5H INT I2,5X,5H INT I2,5X,5H INT I2,5X,5H INT I2,5X,5H INT I
     22,5X,5H INT I2///)
  401 FORMAT(1H1,12H  TIME (SEC),4X,5H ION I2,4X,5H ION I2,4X,5H ION I2,
     1    4X,5H ION I2,4X,5H ION I2,4X,5H ION I2,4X,5H ION I2,4X,5H ION I
     22,5X,5H ION I2///)
      DO 3 L = 4,J
      01 = 001/DNE(L)
      TOTAL = 0.0
      DO 6 K=1,9
      CONC(K) = 01*Y(L,K)
    6 TOTAL = TOTAL + CONC(K)
    3 WRITE(6,200) T(L),(CONC(K),K=1,9),TOTAL,NA
      NC = 1
      NCM = ION
      NCN = 9
      GO TO 950
    2 WRITE(6,401) (KION(K),K=1,9)
      DO 4 L = 4,J
      01 = 001/DNE(L)
      TOTAL = 0.0
      DO 7 K=1,9
      CONC(K) = 01*Y(L,K)
    7 TOTAL = TOTAL + CONC(K)
            ATOTAL(L) = TOTAL
    4 WRITE(6,200) T(L),(CONC(K),K=1,9)
      WRITE(6,201) (KION(K),K=10,18)
      DO 5 L = 4,J
      01 = 001/DNE(L)
            BTOTAL = ATOTAL(L)
      DO 8 K=10,18
      CONC(K) = 01*Y(L,K)
    8       BTOTAL = BTOTAL + CONC(K)
    5 WRITE(6,200) T(L),(CONC(K),K=10, 18),BTOTAL,NA
      NC = 1
      NCM  = 9
      NCN = 9
  950 DO 603 K=NC,NCM
      IF(SFN(K)) 603,603,601
  603 CONTINUE
      GO TO 602
  601 WRITE(6,301) (KION(L),L=NC,NCM)
      L=4
  302 IF(L.GT.J)GO TO 602
      DO 303 K=NC,NCM
      IF(SFN(K)) 304,304,305
  304 XINT(K) = 0.0
      GO TO 303
  305 V = SEX(K)/TE(L)
```

```
          IF(V-0.07) 306,306,307
      306 PP = 0.325*EI(V)
          GO TO 308
      307 PP = 0.2+0.035/V
      308 XINT(K) = 2.01E-25*Y(L,K)*DNE(L)*SFN(K)*EXP(-V)*PP/SQRT(TE(L))
      303 CONTINUE
C
C  IF THE FINE TIME STEP  ´T(L)´ IS EQUAL TO ONE OF THE COARSE TIME
C    STEP THEN REMEMBER IT IN ´THI´ FOR LATER PLOTTING IN THE MAIN PROGRAM.
C
          IF(TIME(TIM).GT.T(L))GO TO 98
       91 DIF1=ABS(TIME(TIM)-T(L))
          T1=T(L)
          GO TO 96
       98 IF (TIM.LT.NTIME)GO TO 99
          IF (L.EQ.J)GO TO 91
       99 DIF2=ABS(TIME(TIM)-T(L))
          DO 100 K=1,ION
      100 THI(TIM,K)=XINT(K)
          T2=T(L)
          WRITE(6,309) T(L),(XINT(K),K=NC,NCM)
     102  L=L+1
          GO TO 302
       96 IF (DIF1.GT.DIF2) GO TO 90
          DO 92 K=1,ION
       92 THI(TIM,K)=XINT(K)
          TTT(TIM)=T1
       94 TIM=TIM+1
          IF(TIM.GT.NTIME)GO TO 102
          GO TO 302
       90 TTT(TIM)=T2
          GO TO 94
      309 FORMAT(E12.4,5X,9E12.4)
      602    IF(ION-NCN)550,550,350
      350    NC = 10
             NCM = ION
             NCN = 18
             GO TO 950
```

```
C
C  AS TIME GOES BY THE LOWER IONS WILL HAVE NO POPULATIONS
C  SO THOSE IONS ARE NOT PURSUED ANY MORE IN SOLVE. (#550TO#82 MAKE THIS HA
C
  550 JA = J - 2
      NAB = NA
      DO 59 K = 1,ION
      KK=K
      IF(Y(JA,K) - YMIN) 59,60,60
   59 CONTINUE
   60 NA = KK
      IF(NAB - NA) 78,82,78
   78 NAM = NA - 1
      IF(NAM) 82,82,81
   81 DO 69 JJ =  1,J
      DO 79 KK = 1,NAM
      Y(JJ,KK) = 1.0
      YR(JJ,KK) = 0.0
   79 CONTINUE
      EPSI(JJ) = 0.0
   69 CONTINUE
   82 RETURN
      END
      FUNCTION EI(X)
C     COMPUTES VALUE OF -EI(-X) WHERE X IS +VE AND LESS THAN 0.1
      Y=X-ALOG(1.781072*X)
      TERM=X
      DO 1 I=2,4
      A=FLOAT(I)
      TERM=TERM*(-X)*(A-1.0)/(A*A)
    1 Y=Y+TERM
      EI=Y
      RETURN
      END
```

PLOT

```
      SUBROUTINE PLOTT(INTE,PFLAG,PFLAG1)
C
C 'PLOTT'  NORMALIZES DATA FOR INTENSITIES AND STORES.SO TELETYPE
C  PLOTTER ROUTINES COULD BE USED FOR PLOTTING AT THE TELETYPE.
C
      INTEGER PFLAG,PFLAG1
C
C  PFLAG &PFLAG1 ARE COUNTERS TO  KNOW WHAT IS  PLOTTED
C
      REAL MAX,INTE
      COMMON J,JMAX,ND,H,DTMAX,NDT,KSTEP,KSEND,END,ED,EH,EN,KDOB,
     1        KHAV1,KHAV2,KHAV3,DOB1,DOB2
      COMMON T(60),EPSI(60), Y(60,18),YR(60,18
     1        ),ANPRIM(18)
      COMMON S(18),ALPHA(18),DENS(100),TEMP(100),TIME(100),SA(18),SB(18)
     1        ,SE(18),NAME(8),KION(18),DNE(60),TE(60),SFN(18),SEX(18)
      COMMON  NTIME,ION,IONM1,NA,NAINI,001,YMIN,YYMIN
      COMMON THI(60,18),TIM,FLAG,F(18),YES(18),W(18),M(5,18),HI(5,18)
     !  ,FLAG1,TTT(60),DIF2,A(18)
      DIMENSION INTE(60,18)
C
C
C
      NT=NTIME-2
      DO 13 K = 1,ION
C FIRST FIND INENSITY MAXIMUM 'MAX' FOR THE ION AND USE IT FOR
C NORMALIZATION
      MAX=0.0
      DO 11 I = 1,NT
   11 IF(INTE(I,K).GT.MAX)MAX=INTE(I,K)
C IF THE MAX IS  0.0 SKIP THAT ION FOR PLOTTING.
      IF(ABS(MAX).LT.1E-10) GO TO 13
      DO 12 I=1,NT
      INTE(I,K)=INTE(I,K)/MAX
  12  IF(ABS(INTE(I,K)).LT.1E-02)INTE(I,K)=0.0
```

```
   13 CONTINUE
      WRITE(7)ION,NT,((TTT(I),INTE(I,K),I=1,NT),K=1,ION),PFLAG,
     1(KION(L),SA(L),SE(L),A(L),L=1,ION),PFLAG1
    7 RETURN
      END
```

V. ACCURACY CHECK

A simple system of two ionic stages is considered. The density and temperature are kept constant. Recombination rates are neglected. The coupled equations are

$$\frac{dN_1}{dt} = - N_1 \, NI_1 \tag{11}$$

$$\frac{dN_2}{dt} = N_1 \, NI_1 - N_2 \, NI_2 \tag{12}$$

The solutions are

$$\frac{N_1}{N_o} = e^{-NI_1 t} \quad ; \quad \frac{N_2}{N_o} = \frac{I_1}{I_1 - I_2} \left[e^{-NI_2 t} - e^{-NI_1 t} \right]$$

The neutral and singly ionized boron in a plasma of constant density ($N = 5\text{x}10^{14} \; /\text{cm}^3$) and temperature ($T = 250$ eV) are considered. The ionization rates for these ions are taken to be

$$I_1 = .7239 \times 10^{-9} \text{ cm}^3/\text{sec and } I_2 = .2344 \times 10^{-7} \text{cm}^3/\text{sec}.$$

A comparison of the results from the analytical solutions given above and the numerical solutions obtained with the code, is shown in Table 1. The maximum difference is less than one percent.

(PTG)

Time (μsec)	N_1/N_o		N_2/N_o	
	Analytical	Code	Analytical	Code
.025	.4045	.4046	.4986	.5049
.05	.1637	.1639	.5735	.5807
.075	.0662	.0664	.5095	.5158
.1	.0268	.0269	.4131	.4183
.125	.0108	.0109	.3216	.3256
.15	.0044	.0044	.2453	.2484

Table 1. Comparison between analytical and numerical solutions.

APPENDIX

1> Plotting on the teletype:

The program TVPLOT together with the subroutines[13] TTPLT1, TTPLTZ and TTPLT3 are listed below. The plotting is done on the teletype and only the time histories of the emission lines from the last four ionization stages could be plotted. Examples of the plots are given in Appendix II.

TVPLOT

```
      INTEGER PFLAG,PFLAG1
      REAL INTE,Y1,Y2,Y3,Y4
      DIMENSION INTE(60,18),TIMEX(60),Y1(60),Y2(60),Y3(60),Y4(60),
     *KION(18),SA(18),SE(18),A(18)
      READ(7)ION,NT,((TIMEX(I),INTE(I,K),I=1,NT),K=1,ION),PFLAG,
     1(KION(L),SA(L),SE(L),A(L),L=1,ION),PFLAG1
      DO 6 I=1,NT
      K=ION
      Y1(I)=INTE(I,K)
      K=K-1
      Y2(I)=INTE(I,K)
      K=K-1
      Y3(I)=INTE(I,K)
      K=K-1
      Y4(I)=INTE(I,K)
    6 CONTINUE
      CALL TTPLOT(TIMEX,NT,30,50,Y1,Y2,Y3,Y4)
C
C IF 'PFLAG' IS SET TO '1' THEN THE TITLE*
C 'EXPERIMENTAL TIME EVOLUTION OF IONS IN A PLASMA'
C SHOULD BE WRITTEN
C
      IF(PFLAG.GT.1)GO TO 100
      WRITE(6,50)
   50 FORMAT(2X,/1X,'EXPERIMENTAL TIME HISTORIES OF EMISSON LINES FROM
     1SUCCESSIVE IONIZATION STAGES IN A PLASMA ')
      GO TO 500
C
C IF 'PFLAG' IS SET TO '2' THEN THE TITLE:
C 'THEORETICAL TIME EVOLUTION OF IONS IN A PLASMA'
C SHOULD BE WRITTEN
C
  100 IF (PFLAG .NE. 2) GOTO 500
      IF (PFLAG1.EQ.1)GO TO 300
      WRITE(6,200)
  200 FORMAT(/12X,'PREDICTED TIME HISTORIES OF EMISSON LINES '/12X,
     1'LOTZ&KUNZE IONIZATION RATE COEFFICIENT WAS USED '/15X,4H ION,5X
     2,2H A,10X,7H E (EV))
      WRITE(6,210)(KION(L),SA(L),SE(L),L=1,ION)
  210 FORMAT(15X,I3,1X,E12.4,1X,F12.4)
      GO TO 500
  300 WRITE(6,310)
  310 FORMAT(2X,//2X,'PREDICTED TIME HISTORIES OF EMISSON LINES '/2X,
     1'E C I P IONIZATION RATE COEFFICIENT (BURGESS&SUMMERS) WAS USED
     2'/15X,4H ION,5X,2H A,10X,7H E (EV))
      WRITE(6,320)(KION(L),A(L),SE(L),L=1,ION)
  320 FORMAT(15X,I3,1X,F10.4,1X,F12.4)
 500   END
```

TTPLT1

```
C
C THIS SUBROUTINE SCALES AND DRAWS PRINTER PLOTS.
C THE SCALING ASSUMES A TELETYPE WIDTH OF 60 LINES FOR THE GRAPH
C AND 10 LINES FOR THE AXIS LABELS--DIFFERENT VALUES CAN BE
C CONJURED UP IF DESIRED.
C
C-----------SUBROUTINE BY B.K.REID NOV.1970--------------------
C
         SUBROUTINE RPLOTR(X,NPTS,LENGTH,WIDTH,NY)
         DIMENSION YY(1500),X(NPTS),AX(2),LINE(63),MARK(4),NMARK(4)
         DIMENSION YMIN(5),YMAX(5),XX(35),YLB(10)
         INTEGER WIDTH,WID,H
         WID=MIN(WIDTH,60)
         NAX=WID//10
         WID=10*NAX
         DATA MARK/'-','+','*','='/
         DATA NMARK/'1','2','3','4'/
         DATA AX/'------','---+'/
C
C ROUND THE WIDTH UP TO A MULTIPLE OF 10 ROWS.
C
         NAXL=(LENGTH-1)//5
         LEN=1+5*NAXL
C
C ROUND THE ELEMENT UP TO A MULTIPLE OF 5 COLUMNS
C
         (I=1,1,I.GT.5,YMIN(I)=1E37,YMAX(I)=-1E37)
         DO 10 I=1,NPTS
C
C WE SCAN THROUGH THE DATA GETTING MINIMUM AND MAXIMUM VALUES
C
         YMAX(1)=MAX(YMAX(1),X(I))
         YMIN(1)=MIN(YMIN(1),X(I))
         DO 10 J=1,NY
         YVAL=YQY(I,J)
```

```
      YMAX(J+1)=MAX(YMAX(J+1),YVAL)
      YMIN(J+1)=MIN(YMIN(J+1),YVAL)
  10  CONTINUE
      NS=NY+1
      DO 101 L=2,NS
      CALL TSCALE(YMIN(L),YMAX(L),YLB,NAX)
      PRINT 899,MARK(L-1),(YLB(H),H=1,NAX+1)
899   FORMAT(1X,A1,8X,6G10.4)
C
C CONVERT MAXIMUM TO SPAN
C
101   CONTINUE
      CALL TSCALE(YMIN(1),YMAX(1),XX,NAXL)
      DO 100 L=1,NS
      YMAX(L)=YMAX(L)-YMIN(L)
      IF(YMAX(L).EQ.0) YMAX(L)=1
100   CONTINUE
      YY(1)=0 @ INITIAL LINK IN COLUMN ZERO.
      IXY=1 @ INITIAL STORE POINTER
C
C  THE DATA HAS BEEN SCALED.  WE NOW WIFFLE THROUGH IT A SECOND
C  TIME AND SET UP THE PLOT ARRAY
C
C
      DO 1001 IXA=1,NPTS
      XV=X(IXA)
      MY=1+LEN*(XV-YMIN(1))/YMAX(1)
      DO 1001 L=1,NY
      M=WID*(YGY(IXA,L)-YMIN(L+1))/YMAX(L+1)
C
C WE ARE GOING TO SEARCH THE PLOTTED-POINT LIST FOR A PLACE TO
C PUT THIS ONE.  THE DATA FORMAT IS:
C
C .....................................................................
C .           .           .                     .                     .
C . SYMBOL    . COLUMN    . ROW (X-AXIS) NO.    . FORWARD LINK BY ROW .
C .           .           .                     .                     .
C .....................................................................
```

```
C
C
      JX=1
      LMMY=MY+(M.LS.12)+(L.LS.18)
1002  CONTINUE
      KX=FLD(24,12,YY(JX)) @ FORWARD LINK
      IF(KX.EQ.0) GO TO 1003
      IF(LMMY.EQ.FLD(0,24,YY(KX))) GO TO 1001
      IF(FLD(12,12,YY(KX)).GT.MY) GO TO 1003
      JX=KX
      GO TO 1002
1003  CONTINUE
C
C WE HAVE FOUND THE CORRECT SPOT IN THE CHAIN FOR THIS
C ITEM--OPEN THE LINK AND INSERT IT.
C
      IXY=IXY+1
      FLD(0,24,YY(IXY))=LMMY
      FLD(24,12,YY(IXY))=KX
      FLD(24,12,YY(JX))=IXY
1001  CONTINUE
      WID=WID+1
      CALL MIMTPL(YY,IXY,XX,LEN)
      RETURN
      SUBROUTINE MIMTPL(Y,NXY,X,NX)
C
C  THIS SUBROUTINE DRAWS A PLOT ON A TELETYPE FOR MIMIC
C
C  Y IS THE ARRAY OF VALUES, INTEGER, RANGE 1-WID
C  MY IS THE NUMBER OF Y VALUES
C  X IS THE ARRAY OF X VALUES
C  NX IS THE NUMBER OF X VALUES, I.E. THE GRAPH LENGTH.
C
C
      DIMENSION X(NX)
      INTEGER Y
      REAL X
      DIMENSION Y(1500)
      PARAMETER NMOD=5
      PRINT 8100,(AX,H=1,NAX)
8100  FORMAT(16X,1H+,6(A6,A4))
      IX=FLD(24,12,Y(1)) @ LINK TO SMALLEST FIRST
      DO 10 I=1,NX
      IXA=I//5
      DO 15 H=1,WID
C
C CLEAR WORKING BUFFER TO ZERO FOR EACH LINE
C
15    LINE(H)=0
809   CONTINUE
      KK=FLD(6,6,Y(IX))+1
      JJ=FLD(0,6,Y(IX))
      MY=FLD(12,12,Y(IX))
      IF(MY.NE.I) GO TO 20
      IF(LINE(KK)) 50,,60
C
C IF THIS IS THE FIRST POINT HERE, JUST STORE IT
C
      LINE(KK)=JJ
      GO TO 21
60    CONTINUE
      LINE(KK)=-2
C
C  IF THERE IS ANOTHER POINT HERE, RECORD THAT
C
      GO TO 21
50    CONTINUE
C
C  AT LEAST 2 OTHER POINTS WERE ON THAT SPOT
C
      LINE(KK)=LINE(KK)-1
21    CONTINUE
      IX=FLD(24,12,Y(IX))
      GO TO 809
20    CONTINUE
      DO 40 J=1,WID
      L=LINE(J)
      M=ABS(L)
      IF(L.GT.0) LINE(J)=MARK(L)
      IF(L.LT.0) LINE(J)=NMARK(M)
      IF(L.EQ.0) LINE(J)=' '
40    CONTINUE
      IF(MOD(I+4,NMOD).EQ.0) PRINT 8900,X(IXA),(LINE(H),H=1,WID)
      IF(MOD(I+4,NMOD).NE.0) PRINT 8901,(LINE(H),H=1,WID)
10    CONTINUE
      PRINT 8100,(AX,H=1,NAX)
      RETURN
8900  FORMAT(G14.4,2H I,61A1)
8901  FORMAT(15X,1HI,61A1)
      END
      END
```

TTPLT2

```
.
.
.   DRIVER FOR TELETYPE PLOT SUBROUTINE.
.
.   THIS SECTION TAKES THE CALL, COUNTS THE ORDINATES, CALLS
.   THE PLOTTING FUNCTION, AND RECEIVES ARGUMENT REQUESTS FOR
.   VALUES FROM THE ORDINATES.
.
.   CALLING SEQUENCE--
.
.   CALL TTPLOT(X,NPTS,LENGTH,WIDTH,Y1,Y2,...,YM)
.
.   X        THE ARRAY OF VALUES OF THE INDEPENDENT VARIABLE
.   NPTS     THE NUMBER OF POINTS OF THE FORM (X,Y(K))
.            (I.E. THE DIMENSION OF X)
.   LENGTH   THE LENGTH OF THE GRAPH IN INTEGER PRINT LINES
.   WIDTH    THE WIDTH OF THE GRAPH IN COLUMNS
.   Y1,Y2    ETC.: THE ARRAYS OF DEPENDENT VALUES
.
.
.   THE POINTS (X,Y1),(X,Y2), ETC. NEED NOT BE IN ANY ORDER, NOR
.   NEED THEY BE EDITED:  THE PLOT SUBROUTINE WILL SORT AND EDIT
.   AUTOMATICALLY.  THE SCALE FACTORS WILL BE COMPUTED BY THE
.   PLOT PROGRAM IN ORDER THAT THE LARGEST POSSIBLE PERCENTAGE OF
.   THE PLOT AREA IS USED BY THE PLOT.
.
.
.
.   NO MORE THAN 4 ORDINATES MAY BE USED IN A GIVEN CALL
.
.
. . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
.
            AXR$
$(1)        LIT.
```

```
TTPLOT*   L,U       A0,4,X11           . COUNT THE ARGUMENTS
          LXI,L     A0,1               . ONE AT A TIME
          TZ,H1     0,A0               . IF IT´S NOT AN ARGUMENT
          TP,XH1    0,A0               . OR AN ALTERNATE RETURN
          JMGI      A0,$-2             . THEN STOP.  ELSE GO.
          AH        A0,(-1,1)          . COMPUTE RETURN ADDRESS
          S,H2      A0,RTN             . TO GO HOME AGAIN
          AN,U      A0,5,X11           . COMPUTE # OF ARGS
          S         A0,NY              . SAVE FOR A RAINY DAY
          LXI,L     X11,4,A0           . LOAD INCREMENT FOR WBACK VALUE
          S         X11,WB+1           . SAVE INDEX 11 FOR ´NEXT´ CALL
          DL        A0,0,X11           . GET X AND NX
          DS        A0,CALL
          DL        A0,2,X11           . GET LENGTH AND WIDTH
          DS        A0,CALL+2          .
          LMJ       X11,RPLOTR         . CALL FORTRAN DRIVE PROG
CALL      RES       4                  . SPACE FOR X,NPTS,LENGTH,WIDTH
          +         NY                 . NUMBER OF Y VALUES
          +         33,WB              . WALKBACK
RTN       J         0                  . RETURN WORD
WB        ´TTPLOT´
          RES       1.
NY        RES       1                  .
.
.
.
.   FUNCTION TO RETURN N´TH  OBSERVATION OF K´TH Y
.
.
.   CALLING SEQLENCE:     X=YQY(N,K)
.
.   THE ALTERNATE RETURN IS TAKEN IF THERE IS NO SUCH VALUE
.
.
YQY*      L         A0,*1,X11          . K
          L         A3,WB+1            . RESTORE CALLING INDEX
          A,U       A3,3,A0            . FIND THE ARGUMENT
          L,H2      A1,,A3             . A1 HAS ARGUMENT BASE ADDR
          A         A1,*0,X11            . FIND THE N+1'TH ENTRY
          AN,U      A1,1                 . AND TEMPER IT DOWN TO N
          L         A0,,A1               . GET THE VALUE OF IT
          J         3,X11.
          END
```

TTPLT3

```
      SUBROUTINE TSCALE(VMIN,VMAX,VSCA,NAXIS)
      DIMENSION VSCA(10)
      LOGICAL NEG
      PARAMETER NSCF=12
C
C
C SUBROUTINE TO SCALE A PLOT.
C
C  THE INPUT VARIABLES
C VMIN AND VMAX CONTAIN THE OBSERVED VALUES OF MINIMUM/MAXIMUM
C VALUES OF THE VARIABLE TO BE SCALED.  ON OUTPUT, THEY WILL
C CONTAIN THE ADJUSTED VALUES TO BE USED FOR 'NICE' NUMBERS
C ALONG THE AXIS OF THE PLOT.
C
C VSCA IS THE ARRAY WHICH WILL CONTAIN AXIS LABELS.  NAXIS IS
C THE NUMBER OF AXIS BLOCKS, SO THAT THERE WILL BE 'NAXIS+1'
C ENTRIES MADE IN VSCA.
C
      DIMENSION XSCF(NSCF)/0.,1.,1.25,1.5,2.,3.,4.,5.,6.,7.5,8.,10./
      NLOOP=0 & LOOP PREVENTER
D     OMIN=VMIN
D     OMAX=VMAX
650   SCF=(VMAX-VMIN)/NAXIS
      DX1=0.
      ZERO=VMIN
      IF(SCF.EQ.0) GO TO 695
      XNC=ALOG10(SCF)
      INC=XNC
      IF(XNC.LE.0.) INC=INC-1
      IF(INC.GT.0) XNC10=10.**INC
      IF(INC.LE.0) XNC10=-(10.**ABS(INC))
      DX=PSCALE(SCF,-XNC10)
      DO 651 ISC=1,NSCF-1
651   IF(DX.GT.XSCF(ISC)) DX1=XSCF(ISC+1)
C
```

```
C A PROBABLE SCALE FACTOR HAS BEEN COMPUTED, AND IT IS 'DX1'
C WE NOW MUST ASSIGN A 'ZERO' TO THE SCALE, AND SEE IF THE
C ASSIGNMENT OF A ROUNDED ZERO IS GOING TO CHANGE THE SCALE
C FACTOR.
C
      IF(VMIN.EQ.0) GO TO 675
      ABMIN=100.0*PSCALE(VMIN,-XNC10)
C
C SCALE THE ZERO TO THE SAME ORDER OF MAGNITUDE AS THE
C INCREMENT, BUT MULTIPLY BY 100 SO THAT .75 AND .25 AND SO
C ON MAY BE KEPT IN INTEGER CONVERSION.
C
      JBMIN=ABS(ABMIN)
      NEG=ABMIN.LT.0
      LAST3=MOD(JBMIN,1000) @ GET LAST 3 DIGITS
      IF(LAST3.LT.0)LAST3=LAST3+1000
      IDELT=DX1*100.0 @ GET 3-DIGIT INCREMENT
      DO 652 ISC=0,8
      LTEST=IDELT*ISC
      IF(LTEST.GT.LAST3) GO TO 653
C
C BACK OFF ON THE LAST THREE DIGITS UNTIL WE COME TO THE
C FIRST SPOT WHICH IS A MULTIPLE OF THE SCALE FACTOR, INCLUDING 0.
C
652   CONTINUE
653   CONTINUE
      IF(.NOT.NEG) LTEST=LTEST-IDELT
C
C  USE THE LARGEST PREVIOUS VALUE FOR POSITIVE SCALING, BUT
C  USE THIS VALUE FOR NEGATIVE SCALING.
C
      JBMIN=JBMIN-LAST3
      ABMIN=(JBMIN+LTEST)/100.
      ZERO=PSCALE(ABMIN,XNC10)
      VMIN=SIGN(ZERO,VMIN)
675   CONTINUE
      DX=DX1
      DX1=NAXIS*DX1
      DX1=PSCALE(DX1,XNC10)
      SPAN=VMIN+DX1
C
C THE SHENANEGANS ABOVE ARE INSERTED TO PREVENT A FLOATING-PT
C TRUNCATION IN CASES WHERE THE SCALE FACTOR IS LESS THAN ONE
C AND NOT EXACTLY REPRESENTABLE IN FLOATING POINT.  FOR EXAMPLE,
C IF THE EVENTUAL INTERVAL IS .1, THEN MULTIPLYING NAXIS BY
C 0.1 WILL NOT GIVE THE SAME ANSWER AS MULTIPLYING NAXIS BY 1
C AND THEN DIVIDING BY 10.  THIS PRECISION IS IMPORTANT.
C
      IF(SPAN.GE.VMAX) GO TO 649
      NLOOP=NLOOP+1
      IF(NLOOP.LE.1) GO TO 650
      PRINT 124
124   FORMAT(' ERROR IN PLOT SCALING ROUTINE:')
D123  FORMAT(1X,A6,1X,G12.5,O13)
D125  FORMAT(1X,A6,1X,I12)
D     PRINT 123,'SPAN',SPAN,SPAN
D     PRINT 123,'VMAX',OMAX,OMAX
D     PRINT 123,'VMIN',OMIN,OMIN
D     PRINT 123,'ZERO',ZERO,ZERO
D     PRINT 123,'XNC10',XNC10,XNC10
D     PRINT 125,'LAST3',LAST3
D     PRINT 125,'IDELT',IDELT
D     PRINT 125,'LTEST',LTEST
D     PRINT 125,'JBMIN',JBMIN
D     PRINT 123,'DX1',DX1,DX1
649   CONTINUE
      VMAX=SPAN
695   CONTINUE
      DX=PSCALE(DX,XNC10)
      DO 655 IH=1,NAXIS+1
      VSCA(IH)=VMIN+(IH-1)*DX
655   CONTINUE
      RETURN
C
C
C FUNCTION TO SCALE BY EXPONENTIAL SCALE FACTOR
```

```
C
      FUNCTION PSCALE(MANTIS,CHARAC)
      REAL MANTIS
      IF(CHARAC.GT.0) PSCALE=MANTIS*CHARAC
      IF(CHARAC.LT.0) PSCALE=MANTIS/ABS(CHARAC)
      RETURN
      END
      END
```

APPENDIX II

Determination of ionization rate coefficients:

One possible use of this code as mentioned earlier, is to determine ionization rate coefficients. This involves changing the ionization rate coefficients in the coupled rate equations until the predicted time histories match with the experimentally observed time histories. What is thus measured is therefore an effective ionization rate, i.e. a sum of the ionization rates from the ground state, including inner-shell ionization, and all the populated excited states. A detailed description of this method was given in Ref. 2. Another useful result in matching the time histories is that the percentage composition of the various ionization stages at any instant of time would also be predicted.

In using the procedure for the determination of ionization rates the following points are to be carefully considered.

1.) As we are theoretically predicting the time histories we should carefully evaluate how critically all these predictions depend on initial conditions i.e., degree of ionization, electron density and temperature at early times. As we know, it is very difficult to be accurate about such initial conditions. So the earlier ionization stages may not be considered for measurements. The ionization rate coefficients of these ions could be adjusted until the decay of an emission line from at least one ion prior to the ion under consideration would match with the experiment. This should also make the early part of the emission from the ion under consideration match with the experiment. Thus the initial conditions could be fixed for the ions under consideration.

2.) The electron density N and the temperature T should be spatially non-varying so that ionization proceeds uniformly in the plasma under observation and the modelling of the plasma in Eq. (3) would be perfect.

3.) Also, the electron density and temperature at the time of occurrence of the ions under consideration should ideally be non-varying in time for a good determination of ionization rates.[1] However, some variations of N and T can be accounted for. As was discussed in Ref. 2, the first three terms in Eq. (7), Ref. 2 should not dominate the time history.

4.) It is important to select and obtain the time histories of emission lines connecting to the ground state which are not self-absorbed.

As an example, the determination of the ionization rate coefficient for C V (He-like carbon) is considered from an experiment on the 15 KJ Θ-pinch.[5] The density and temperature profiles for this plasma condition obtained by the laser scattering technique are given in Fig. 1. Experimentally observed time histories of emission lines from C IV, C V, and C VI are given in Fig. 2. The predicted time histories that are matched to the experimental ones are given in Fig. 3 and Fig. 4 using Lotz and Kunze ionization rate coefficients and Burgess and Summers ionization rate coefficients, respectively, which yielded the same results. The effective ionization rate coefficient thus determined was 0.8 x 10^{-10} cm^3/sec at an electron temperature of 200 ev and a density of 4.95 x 10^{15} /cm^3. The corresponding estimate for the theoretical ionization rate, both by semiempirical and semiclassical methods after including the effect of the metastable state (1s2p (^3S)) ionization agrees with the experiment. The matching of time histories was sensitive enough to show a significant difference if the C V ionization rate is varied by ±25%.

DATA INPUT TO THE COMPUTER*

```
CARBØN, 11 MTØRR
     6     37       1        2        1
                1     0.53E-08     3.00E 00      1.13E 01      5.00E 07   DATA
                2     0.20E-09     3.00E 00      2.44E 01      1.00E 00   for Lotz &
                3     0.75E-09     3.00E 00      4.79E 01      1.00E 00   Kunze Ioniza-
                4     0.13E-09     3.00E 00      6.45E 01      1.00E 00   tion rates.
                5     5.00E-10     3.00E 00      3.92E 02      1.00E 00
                6     2.04E-10     3.00E 00      4.90E 02      1.00E 00
  50    6     2     10000 1.0E+00 1.0E-03 1.0E-01 1.0E+00 2.5E-03
   -0.10E-06      2.50E 01     0.00E 00
    0.00E 00      2.50E 01     0.50E 15
    0.10E-06      3.50E 01     1.00E 15          Experimentally obtained
    0.20E-06      3.50E 01     1.50E 15          electron temperature and
    0.30E-06      3.50E 01     1.50E 15          electron density profiles
    0.40E-06      3.50E 01     1.90E 15
    0.50E-06      0.90E 02     1.90E 15
    0.60E-06      1.05E 02     1.90E 15
    0.70E-06      1.16E 02     1.90E 15
    0.80E-06      1.23E 02     2.00E 15
    0.90E-06      1.32E 02     2.50E 15
    1.00E-06      1.40E 02     3.00E 15
    1.10E-06      1.62E 02     3.50E 15
    1.20E-06      1.88E 02     4.00E 15
    1.30E-06      2.20E 02     4.20E 15
    1.40E-06      2.20E 02     4.25E 15
    1.50E-06      2.20E 02     4.35E 15
    1.60E-06      2.20E 02     4.35E 15
    1.70E-06      2.20E 02     4.35E 15
    1.80E-06      2.20E 02     4.35E 15
    1.90E-06      2.19E 02     4.35E 15
    2.00E-06      2.18E 02     4.30E 15
    2.10E-06      2.17E 02     4.25E 15
    2.20E-06      2.15E 02     4.25E 15
    2.30E-06      2.14E 02     4.20E 15
    2.40E-06      2.13E 02     4.15E 15
    2.50E-06      2.11E 02     4.10E 15
    2.60E-06      2.06E 02     4.05E 15
    2.70E-06      2.00E 02     4.00E 15
    2.80E-06      1.85E 02     3.95E 15
    2.90E-06      1.82E 02     3.80E 15
    3.00E-06      1.60E 02     3.65E 15
    3.10E-06      1.46E 02     3.50E 15
    3.20E-06      1.32E 02     3.35E 15
    3.30E-06      1.19E 02     3.05E 15
    3.40E-06      1.06E 02     2.70E 15
    3.50E-06      0.96E 02     2.30E 15
     0            0                                      DATA for excitation
     0            0

    0.2        39.68
    0.65      307.89
    1.0       367.5

    10      9.3                                          DATA FOR
    10     12.7                                          dielectronic
     3      8.0                                          recombination
  1  2    307.9
  1  1    367.0
.400   E+00 2.8298 E+01 2.1293 E+02                               (P.T.O)
```

*For details, see-read statements in MAIN-R/W.

```
.400   E+00 2.8293 E+01 2.1293 E-02
.140   E+00 1.24376E+02 2.31397E+02
.400   E+00 2.47364E+02
.020   E+01 1.64476E+02
.130   E+01 2.39199E+03
.130   E+01 1.4398 E+03
```

DATA for Burgess and Summers (E.C.I.P.) ionization rates.

```
01
05
11
19
27
34   05   00
37   095
39   14
40   17
39   245   15
37   30     2
32   325    3
28   36   10
23   38   145
19   39   19
15   40   23
12   40   265
10   39   30
 8   38   33
 6   37   35
 5   35   36
 4   33   38
 3   30   395
 2   265  40
 1   235  40
 1   20   40
     18   375
     15   345
     13   315
     11   27
      9   23
*
*
```

Digitized data for the experimental time histories of emission lines from C IV, C V and C VI.

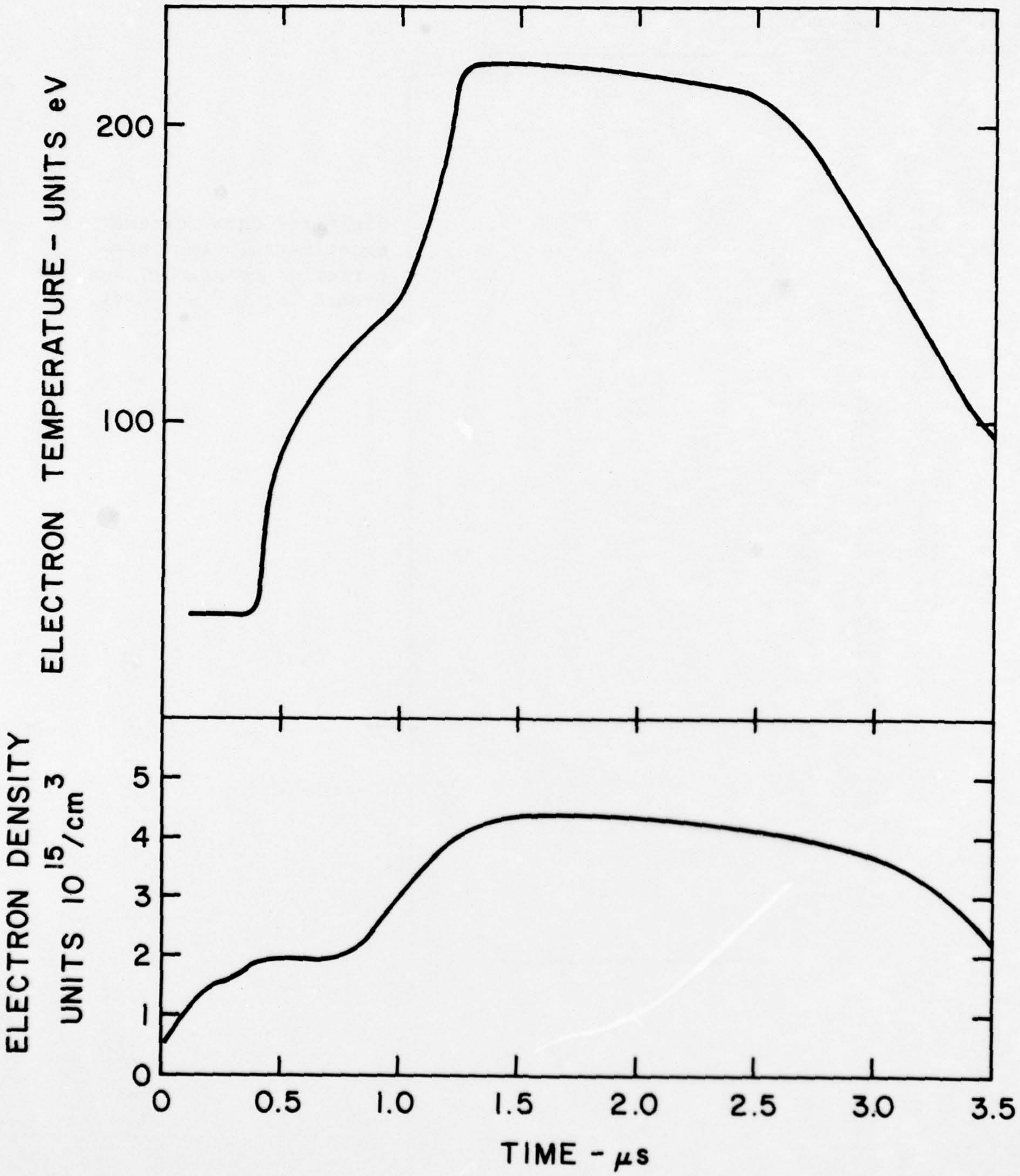


Fig. 1 ELECTRON DENSITY AND TEMPERATURE PROFILES (2% CARBON IN 11 mTorr H_2 CASE)

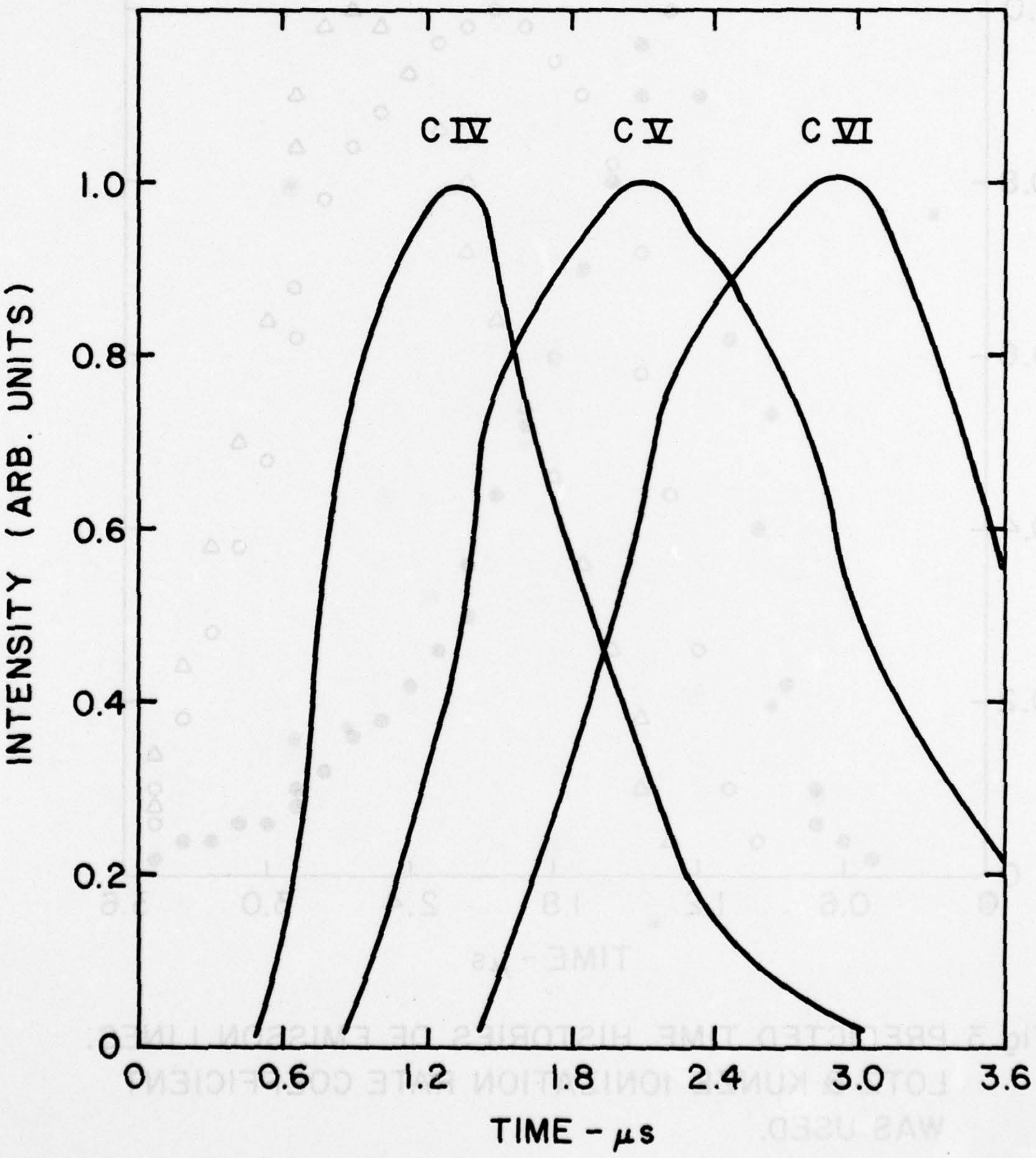


Fig. 2 EXPERIMENTAL TIME HISTORIES OF EMISSION LINES FROM SUCCESSIVE IONIZATION STAGES IN A PLASMA

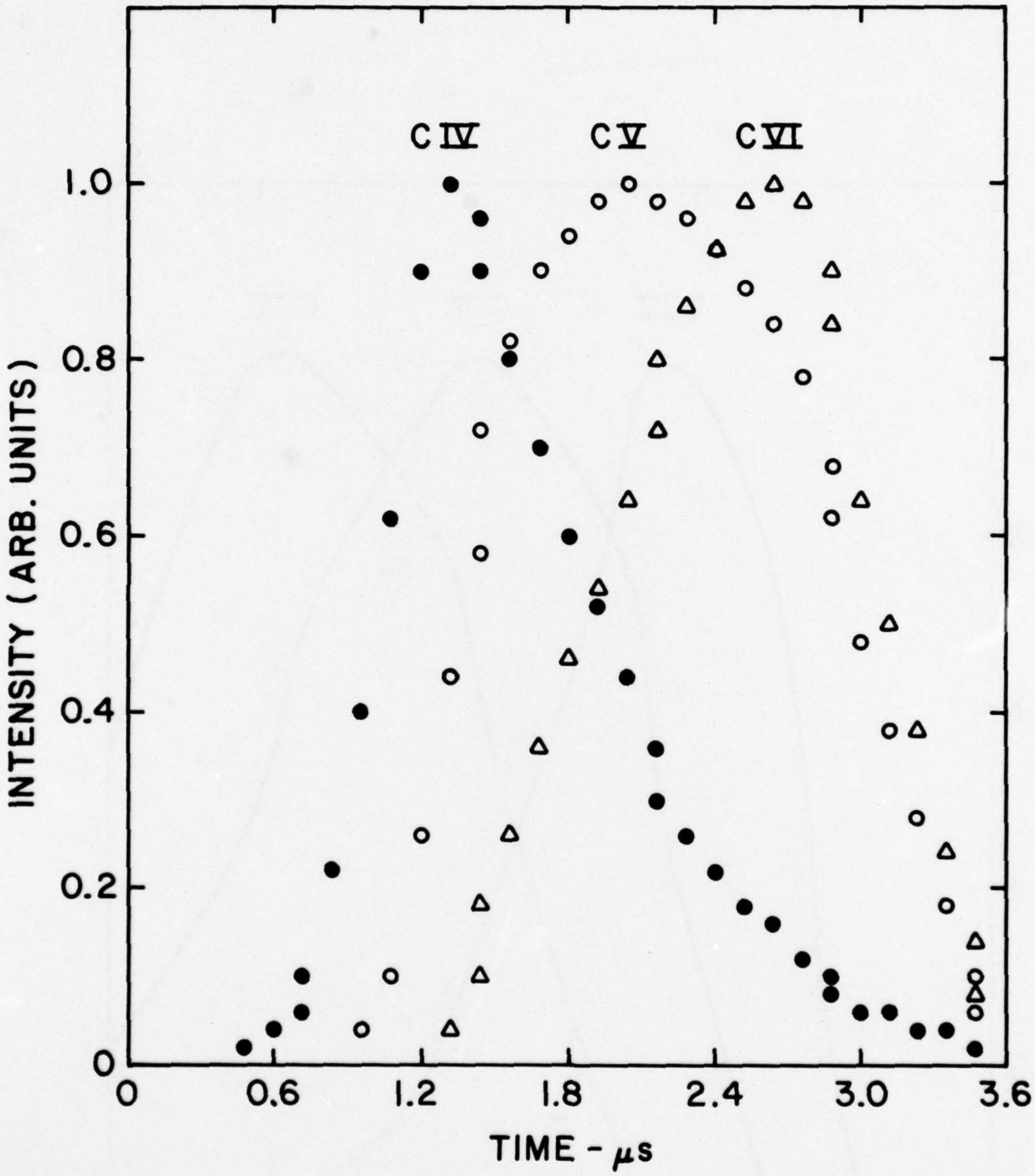


Fig. 3 PREDICTED TIME HISTORIES OF EMISSON LINES. LOTZ & KUNZE IONIZATION RATE COEFFICIENT WAS USED.

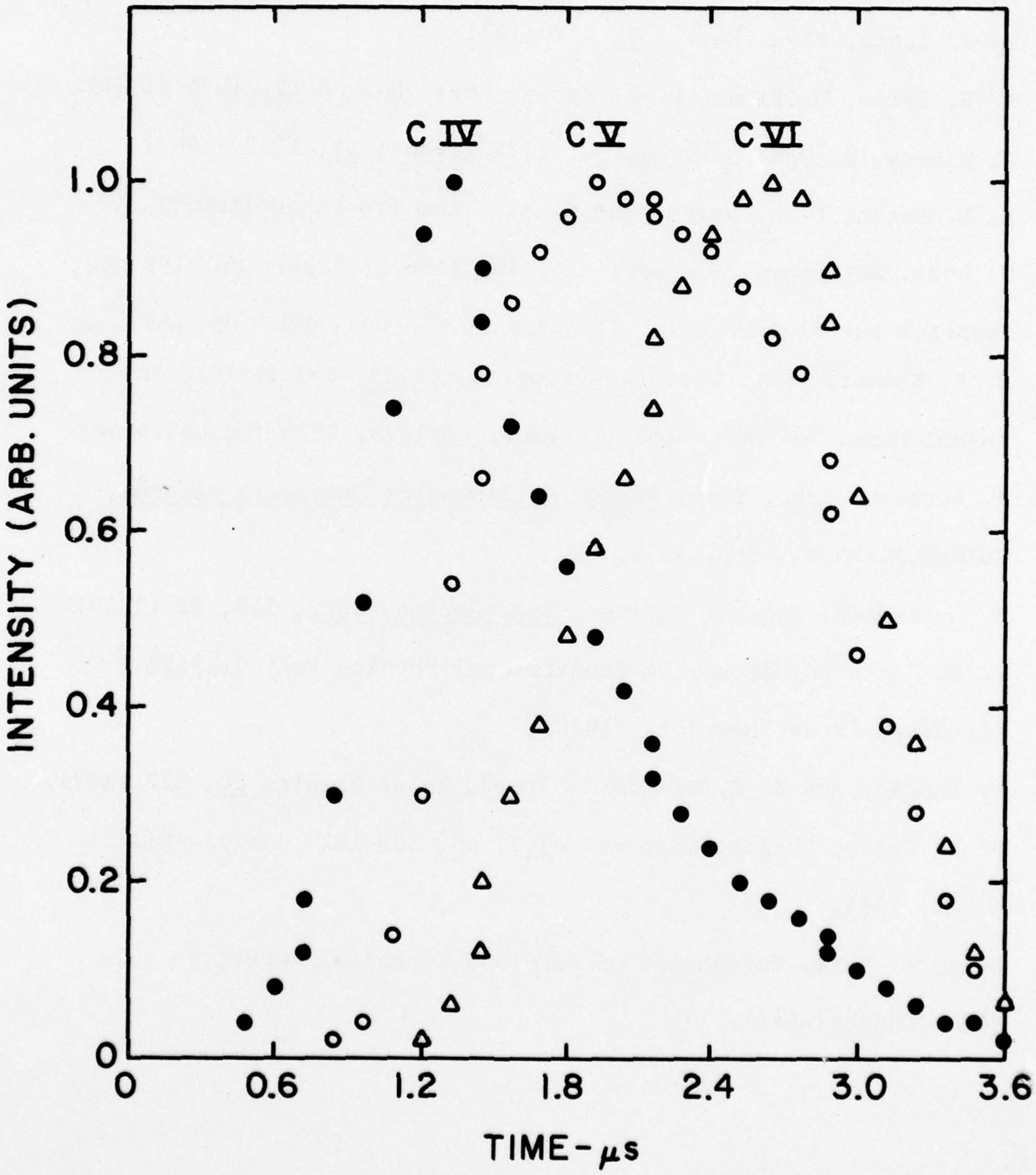


Fig. 4 PREDICTED TIME HISTORIES OF EMISSION LINES, ECIP IONIZATION RATE COEFFICIENT (BURGESS & SUMMERS) WAS USED.

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